Welcome to STN International Web Page URLs for STN Seminar Schedule - N. America NEWS 1 "Ask CAS" for self-help around the clock NEWS 3 May 10 PROUSDDR now available on STN NEWS NEWS 4 May 19 PROUSDDR: One FREE connect hour, per account, in both May and June 2004 NEWS 5 May 12 EXTEND option available in structure searching NEWS 6 May 12 Polymer links for the POLYLINK command completed in REGISTRY NEWS 7 May 17 FRFULL now available on STN New UPM (Update Code Maximum) field for more efficient patent NEWS 8 May 27 SDIs in CAplus NEWS 9 May 27 CAplus super roles and document types searchable in REGISTRY NEWS 10 May 27 Explore APOLLIT with free connect time in June 2004 Jun 22 STN Patent Forums to be held July 19-22, 2004 NEWS 11 NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004 STN Operating Hours Plus Help Desk Availability NEWS HOURS General Internet Information NEWS INTER Welcome Banner and News Items NEWS LOGIN Direct Dial and Telecommunication Network Access to STN NEWS PHONE CAS World Wide Web Site (general information) NEWS WWW

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004

=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

COPYRIGHT (C) 2004 American Chemical Society (ACS)

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> file casreact
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 10.08 10.29

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 20 Jun 2004 VOL 140 ISS 25

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See <u>HELP SLIMIT</u> for the new, higher limits.

=> L1 STRUCTURE UPLOADED

=> 11

L1 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d 11 L1 HAS NO ANSWERS L1 STR

=> s 11
SAMPLE SEARCH INITIATED 09:44:20 FILE 'CASREACT'
SCREENING COMPLETE - 6 REACTIONS TO VERIFY FROM

6 DOCUMENTS

100.0% DONE 6 VERIFIED 0 HIT RXNS SEARCH TIME: 00.00.01

0 DOCS

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 6 TO
                                         266
PROJECTED ANSWERS:
                            0 TO
       0 SEA SSS SAM L1 ( 0 REACTIONS)
L2
=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:44:25 FILE 'CASREACT'
SCREENING COMPLETE - 389 REACTIONS TO VERIFY FROM 78 DOCUMENTS
                                                               0 DOCS
                                O HIT RXNS
100.0% DONE 389 VERIFIED
SEARCH TIME: 00.00.01
          O SEA SSS FUL L1 ( O REACTIONS)
L3
=>
     STRUCTURE UPLOADED
=> d 14
L4 HAS NO ANSWERS
L4
               STR
=> s 14
SAMPLE SEARCH INITIATED 09:45:43 FILE 'CASREACT'
                         6 REACTIONS TO VERIFY FROM
                                                       6 DOCUMENTS
SCREENING COMPLETE -
100.0% DONE 6 VERIFIED 0 HIT RXNS
                                                               0 DOCS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                       BATCH **COMPLETE**
                             6 TO
                                         266
PROJECTED VERIFICATIONS:
                                O TO
PROJECTED ANSWERS:
                                           0
             O SEA SSS SAM L4 ( O REACTIONS)
L5
=> s 14 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:45:48 FILE 'CASREACT'
                       389 REACTIONS TO VERIFY FROM
                                                      78 DOCUMENTS
SCREENING COMPLETE -
                                                               3 DOCS
                                89 HIT RXNS
100.0% DONE
              389 VERIFIED
SEARCH TIME: 00.00.01
             3 SEA SSS FUL L4 ( 89 REACTIONS)
L6
=> d 16, ibib abs crd, 1-3
                   CASREACT COPYRIGHT 2004 ACS on STN
     ANSWER 1 OF 3
L6
           Citing
   Full
         References
   Text
```

139:301299 CASREACT

ACCESSION NUMBER:

TITLE:

Structure-Activity Relationships of the p38 α MAP Kinase Inhibitor 1-(5-tert-Butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-yl-ethoxy)naph-

thalen-1-yl]urea (BIRB 796)

Regan, John; Capolino, Alison; Cirillo, Pier F.; AUTHOR (S):

Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Kroe, Rachel R.; Madwed, Jeffrey; Moriak, Monica; Nelson, Richard; Pargellis, Christopher A.; Swinamer,

Alan; Torcellini, Carol; Tsang, Michele; Moss, Neil

Department of Medicinal Chemistry, Boehringer CORPORATE SOURCE:

Ingelheim Pharmaceuticals Research and Development

Center, Ridgefield, CT, 06877, USA

Journal of Medicinal Chemistry (2003), 46(22),

4676-4686

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER:

SOURCE:

American Chemical Society

DOCUMENT TYPE:

Journal

English LANGUAGE:

We report on the structure-activity relationships (SAR) of AB 1-(5-tert-butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-ylethoxy)naphthalen-1-yl]urea (BIRB 796), an inhibitor of p38 α MAP kinase which has advanced into human clin. trials for the treatment of autoimmune diseases. Thermal denaturation was used to establish mol. binding affinities for this class of p38\alpha inhibitors. The tert-Bu group remains a crit. binding element by occupying a lipophilic domain in the kinase which is exposed upon rearrangement of the activation loop. arom. ring attached to N-2 of the pyrazole nucleus provides important π -CH2 interactions with the kinase. The role of groups attached through an ethoxy group to the 4-position of the naphthalene and directed into the ATP-binding domain is elucidated. Pharmacophores with good hydrogen bonding potential, such as morpholine, pyridine, and imidazole, shift the melting temp. of $p38\alpha$ by 16-17° translating into Kd values of 50-100 pM. Finally, we describe several compds. that potently inhibit $TNF-\alpha$ prodn. when dosed orally in mice.

- RX(33) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(34) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(35) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(36) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(37) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(55) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(56) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(57) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(60) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(62) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(63) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(64) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(66) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(76) OF 120 REACTION DIAGRAM NOT AVAILABLE

```
RX(85) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(86) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(87) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(89) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(90) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(91) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(93) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(94) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(95) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(98) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(99) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(100) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(101) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(102) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(111) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(116) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(117) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(118) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(119) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(120) OF 120 - REACTION DIAGRAM NOT AVAILABLE
                               THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
                         33
REFERENCE COUNT:
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
      ANSWER 2 OF 3 CASREACT COPYRIGHT 2004 ACS on STN
 L6
ACCESSION NUMBER:
                         138:24709 CASREACT
                         Preparation of pyrazole compds. and bis
TITLE:
                         pyrazole-1H-pyrazole intermediates as antiinflammatory
                         agents
                         Kapadia, Suresh R.; Song, Jinhua J.; Yee, Nathan K.
INVENTOR(S):
                         Boehringer Ingelheim Pharmaceuticals, Inc., USA
PATENT ASSIGNEE(S):
                         U.S., 37 pp., Cont.-in-part of U.S. 6,372,773.
SOURCE:
                         CODEN: USXXAM
                         Patent
DOCUMENT TYPE:
                         English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
                         3
PATENT INFORMATION:
                                           APPLICATION NO. DATE
     PATENT NO.
                      KIND
                            DATE
```

20020205

US 2002-67492

20021210

B1

US 6492529

US	6319921	B1	20011120	US	2000-484638	20000118
US	6333325	B1	20011225	US	2001-871559	20010531
US	6329415	B1	20011211	US	2001-891579	20010626
US	2002065285	A1	20020530	US	2001-891820	20010626
US	6506748	B2	20030114			
US	6372773	B1	20020416	US	2001-920899	20010802
PRIORITY	Y APPLN. INFO.:			US	2000-484638	20000118
				US	2001-920899	20010802
				US	1999-116400P	19990119
				US	2001-891579	20010626
OTHER SO	OURCE(S):	MAI	RPAT 138:24709			

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Pyrazole compds., e.g. I, as well as bis pyrazole-1H-pyrazole intermediate compds. e.g. II, were prepd. The compds. are useful in pharmaceutic compns. for treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases. All prepd. compds. had IC50 < 10 mM for inhibition of TNF.alpha. in lipopolysaccharide stimulated THP cells.

RX(74) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(79) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(82) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(84) OF 282 - 2 STEPS

1. HCl, Dioxane 2. EtN(Pr-i)2, DMSO

RX(84) OF 282 - 2 STEPS

RX(93) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(95) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(96) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(97) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(98) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(105) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(134) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(136) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(141) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(143) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(145) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(147) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(148) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(149) OF 282 - 3 STEPS

1. BrCH2CH2Cl, K2CO3,

MeCN

2. HCl. Dioxane

RX(149) OF 282 - 3 STEPS

1. HCl, Dioxane 2. EtN(Pr-i)2, DMSO 3. NaI, Me2CO

RX(151) OF 282 - 3 STEPS

RX(152) OF 282 - 4 STEPS

1. BrCH2CH2Cl, K2CO3,
MeCN
2. HCl, Dioxane
3. EtN(Pr-i)2, DMSO
4. NaI, Me2CO

RX(152) OF 282 - 4 STEPS

RX(155) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(156) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(164) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(166) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(167) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(168) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(169) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(170) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(175) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(176) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(177) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(178) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(179) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(180) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(181) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(192) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(194) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(230) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(231) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(234) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(235) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(238) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(239) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(243) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(244) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(245) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(246) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(247) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(251) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(252) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(253) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(254) OF 282 - REACTION DIAGRAM NOT AVAILABLE

5

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CASREACT COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

SOURCE:

ACCESSION NUMBER: 137:119059 CASREACT

TITLE: Pyrazole Urea-Based Inhibitors of p38 MAP Kinase: From

Lead Compound to Clinical Candidate

AUTHOR(S): Regan, John; Breitfelder, Steffen; Cirillo, Pier;

Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Klaus, Bernhard; Madwed, Jeffrey; Moriak, Monica;

Moss, Neil; Pargellis, Chris; Pav, Sue; Proto, Alfred;

Swinamer, Alan; Tong, Liang; Torcellini, Carol

CORPORATE SOURCE: Research and Development Center, Department of

Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA Journal of Medicinal Chemistry (2002), 45(14),

2994-3008

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB We report on a series of N-pyrazole, N'-aryl ureas and their mode of binding to p38 mitogen activated protein kinase. Importantly, a key binding domain that is distinct from the ATP (ATP) binding site is exposed when the conserved activation loop, consisting in part of Asp168-Phe169-Gly170, adopts a conformation permitting lipophilic and hydrogen bonding interactions between this class of inhibitors and the protein. We describe the correlation of the structure-activity relationships and crystallog. structures of these inhibitors with p38. In addn., we incorporated another binding pharmacophore that forms a hydrogen bond at the ATP binding site. This modification affords significant improvements in binding, cellular, and in vivo potencies resulting in the selection of Compd. 45 (BIRB 796) as a clin. candidate for the treatment of inflammatory diseases.

RX(67) OF 99 - REACTION DIAGRAM NOT AVAILABLE

RX(86) OF 99 - REACTION DIAGRAM NOT AVAILABLE

-1.98

-1.98

RX(88) OF 99 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

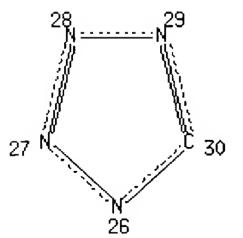
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> L7 STRUCTURE UPLOADED

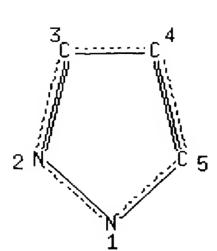
=> d 17 L7 HAS NO ANSWERS L7 STR

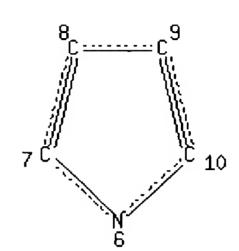
CA SUBSCRIBER PRICE

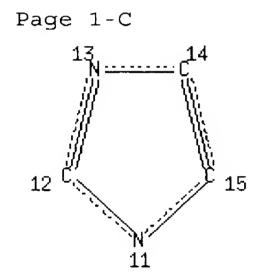


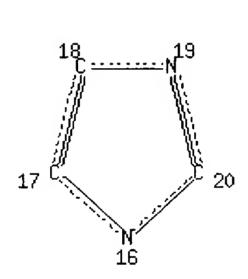
Page 1-A

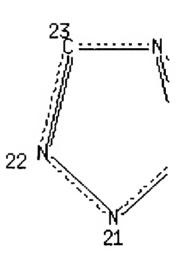
=



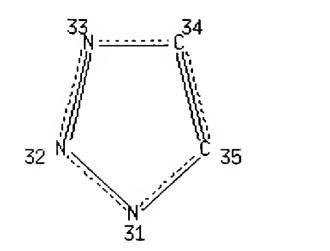




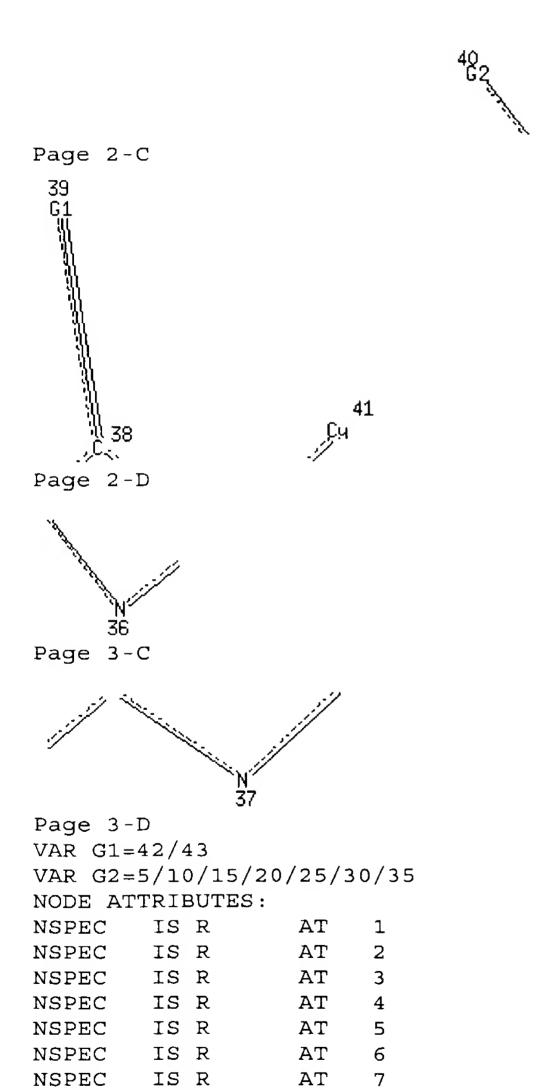




Page 1-D 24



PRO



NSPEC

NSPEC

NSPEC

IS R

IS R

IS R

AT

AT

AT

8

9

10

```
IS R
NSPEC
                     AT
                         11
         IS R
NSPEC
                     AT
                         12
NSPEC
         IS R
                     AT
                         13
NSPEC
         IS R
                     AT
                         14
NSPEC
         IS R
                     AT
                         15
NSPEC
         IS R
                     AT
                         16
NSPEC
         IS R
                     AT
                         17
NSPEC
         IS R
                     AT
                         18
NSPEC
                         19
         IS R
                     AT
NSPEC
         IS R
                         20
                     AT
                         21
NSPEC
         IS R
                     AT
NSPEC
         IS R
                         22
                     AT
         IS R
                         23
NSPEC
                     AT
NSPEC
         IS R
                     AT
                         24
NSPEC
         IS R
                     AT
                         25
NSPEC
         IS R
                     AT
                         26
NSPEC
         IS R
                     AT
                         27
NSPEC
         IS R
                     AT
                         28
                         29
NSPEC
         IS R
                     AT
NSPEC
         IS R
                     AT
                         30
         IS R
NSPEC
                     AT
                         31
NSPEC
         IS R
                         32
                     AT
NSPEC
         IS R
                     AT
                         33
NSPEC
         IS R
                     AT
                         34
                         35
NSPEC
         IS R
                     AT
NSPEC
         IS C
                         36
                     AT
NSPEC
         IS C
                     AT
                         37
         IS C
                         38
NSPEC
                     AT
         IS C
                    AT
NSPEC
                         39
         IS C
NSPEC
                    AT
                         40
NSPEC
         IS C
                     AT
                         41
DEFAULT MLEVEL IS ATOM
                         36 37 38 42 43
MLEVEL
         IS CLASS
                    AT
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE

SINCE FILE	TOTAL
ENTRY	SESSION
0.84	228.38
SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.98
	ENTRY 0.84 SINCE FILE ENTRY

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004 L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004

=> s 17/prep

QUALIFICATION NOT VALID FOR L7

Field code qualifications can only be applied to text terms.

=> s 17

SAMPLE SEARCH INITIATED 09:48:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 763 TO ITERATE

100.0% PROCESSED 763 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

PROJECTED ITERATIONS: 13603 TO 16917
PROJECTED ANSWERS: 1081 TO 2159

L8 50 SEA SSS SAM L7

=> s 17 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y FULL SEARCH INITIATED 09:48:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 15438 TO ITERATE

100.0% PROCESSED 15438 ITERATIONS

1575 ANSWERS

SEARCH TIME: 00.00.01

L9 1575 SEA SSS FUL L7

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

155.42 383.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE

0.00 -1.98

FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 19/prep

312 L9

3163220 PREP/RL

L10

225 L9/PREP

(L9 (L) PREP/RL)

=> file reg

CA SUBSCRIBER PRICE

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
2.36 386.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

ENTRY

0.00

SESSION

-1.98

FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

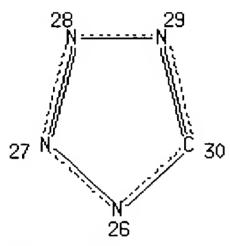
=>

L11 STRUCTURE UPLOADED

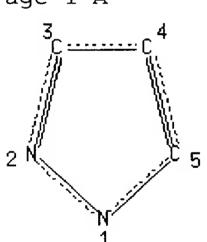
=> d 111

L11 HAS NO ANSWERS

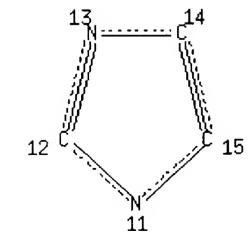
L11 STR

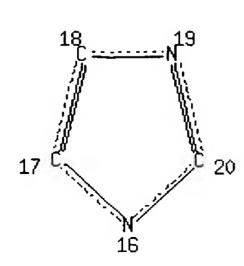


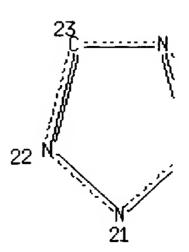
Page 1-A

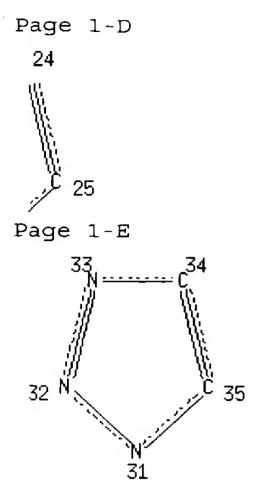


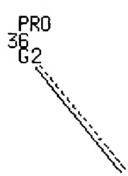
Page 1-C











Page 2-C



Page 3-C VAR G2=5/10/15/20/25/30/35

NODE ATTRIBUTES:

NSPEC	IS	R		ΑT	1
NSPEC	IS	R		ΑT	2
NSPEC	IS	R		ΑT	3
NSPEC	IS	R		ΑT	4
NSPEC	IS	R		ΑT	5
NSPEC	IS	R		AT	6
NSPEC	IS	R		AT	7
NSPEC	IS	R		\mathtt{AT}	8
NSPEC	IS	R		ΑT	9
NSPEC	IS	R		AT	10
NSPEC	IS	R		ΑT	11
NSPEC	IS	R		\mathtt{AT}	12
NSPEC	IS	R		\mathtt{AT}	13
NSPEC	IS	R		\mathbf{AT}	14
NSPEC	IS	R	i	AT	15
NSPEC	IS	R	1	TA	16
NSPEC	IS	R	i	TA	17
NSPEC	IS	R	i	AΤ	18
NSPEC	IS	R	7	TA	19
NSPEC	IS	R	7	ΣТ	20

```
NSPEC
          IS R
                       AT 21
NSPEC
          IS R
                       AT
                            22
NSPEC
          IS R
                           23
                       AT
NSPEC
          IS R
                       AT
                            24
NSPEC
          IS R
                       AT
                            25
NSPEC
          IS R
                       \mathsf{AT}
                           26
NSPEC
          IS R
                       AT
                            27
          IS R
NSPEC
                      \mathtt{AT}
                           28
          IS R
NSPEC
                       \mathtt{AT}
                            29
NSPEC
          IS R
                       AT
                            30
NSPEC
          IS R
                      \mathtt{AT}
                           31
NSPEC
          IS R
                      \mathtt{AT}
                            32
NSPEC
          IS R
                      AT
                            33
NSPEC
          IS R
                      \mathtt{AT}
                           34
NSPEC
          IS R
                      \mathsf{AT}
                            35
          IS C
NSPEC
                      AT
                            36
NSPEC
          IS C
                      AT
                            37
DEFAULT MLEVEL IS ATOM
        IS CLASS
MLEVEL
                     \mathtt{AT}
                           37
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

=> s 111

SAMPLE SEARCH INITIATED 09:51:08 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 28473 TO ITERATE

3.5% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

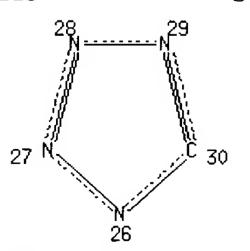
PROJECTED ITERATIONS: 559379 TO 579541 PROJECTED ANSWERS: 117185 TO 126543

L12 50 SEA SSS SAM L11

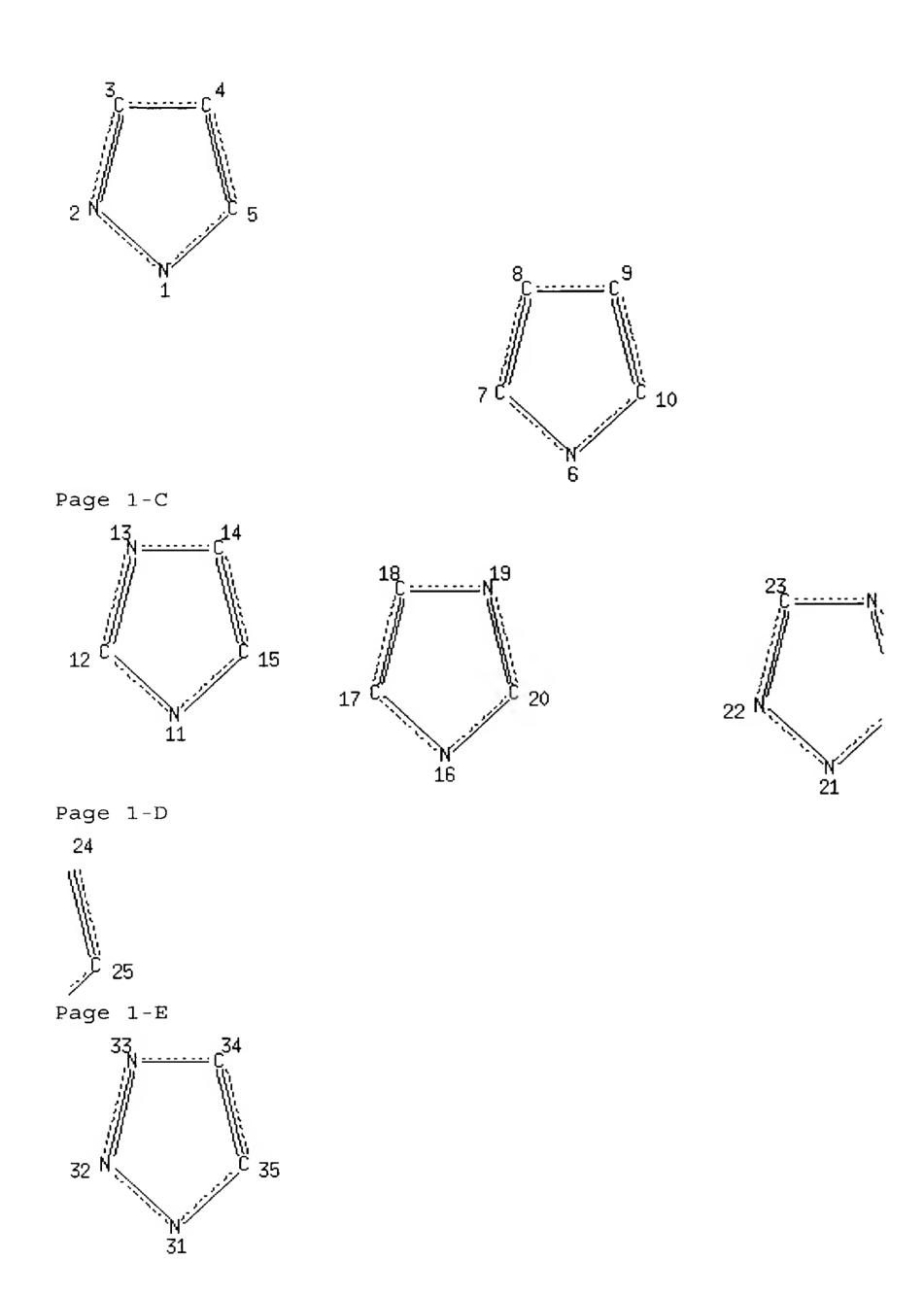
=> L13 STRUCTURE UPLOADED

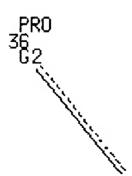
=> d 113

L13 HAS NO ANSWERS
L13 STR

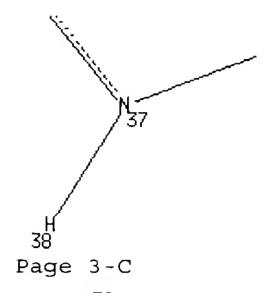


Page 1-A





Page 2-C



Page 3-D VAR G2=5/10/15/20/25/30/35

	,	•	•
NODE	ATTRI	BUT	TES:

NODE AT	TRI	BUTES:				
NSPEC	IS	R	TA	1		
NSPEC	IS	R	AT	2		
NSPEC	IS	R	AT	3		
NSPEC	IS	R	\mathtt{AT}	4		
NSPEC	IS	R	AT	5		
NSPEC	IS	R	\mathtt{AT}	6		
NSPEC	IS	R	$\mathbf{T}\mathbf{A}$	7		
NSPEC	IS	R	\mathtt{AT}	8		
NSPEC	IS	R	\mathtt{AT}	9		
NSPEC	IS	R	\mathtt{AT}	10		
NSPEC	IS	R	\mathtt{AT}	11		
NSPEC	IS	R	AT	12		
NSPEC	IS	R	$\mathbf{T}\mathbf{A}$	13		
NSPEC	IS	R	\mathtt{AT}	14		
NSPEC	IS	R	AT	15		
NSPEC	IS	R	TA	16		
NSPEC	IS	R	AT	17		
NSPEC	IS	R	AT	18		
NSPEC	IS	R	AT	19		
NSPEC	IS	R	TA	20		
NSPEC	IS	R	AT	21		
NSPEC	IS	R	TA	22		
NSPEC	IS	R	AT	23		
NSPEC	IS	R	AT	24		
NSPEC	IS	R	AT	25		
NSPEC	IS	R	AT	26		
NSPEC	IS	R	AT	27		
NSPEC	IS	R	AT	28		
NSPEC	IS	R	\mathtt{AT}	29		
NSPEC	IS	R	AT	30		
NSPEC	IS	R	AT	31		
NSPEC	IS	R	AT	32		
NSPEC	IS	R	AT	33		
NSPEC	IS	R	AT	34		
NSPEC	IS	R	AT	35		
NSPEC	IS	C	AT	36		
NSPEC	IS		AT	37		
NSPEC			AT	38		
	IS		ΑT			
DEFAULT					_	
MLEVEL						39
DEFAULT	ECI	LEVEL IS	S LI	MITE	ED	

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE

=> s 113

SAMPLE SEARCH INITIATED 09:51:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 28473 TO ITERATE

3.5% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

49 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

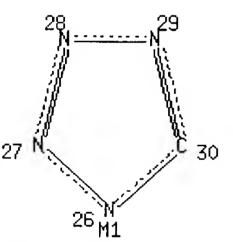
PROJECTED ITERATIONS: 559379 TO 579541

PROJECTED ANSWERS: 25663 TO 30143

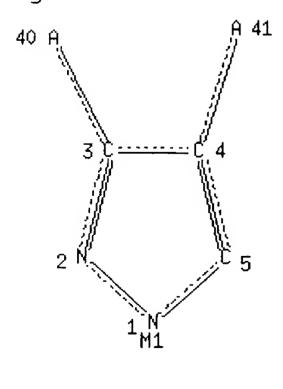
L14 49 SEA SSS SAM L13

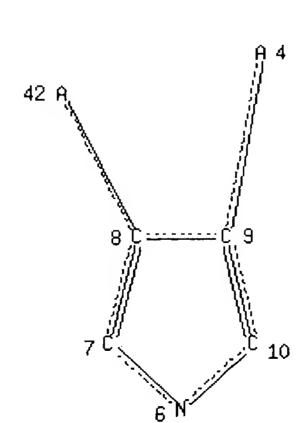
=> L15 STRUCTURE UPLOADED

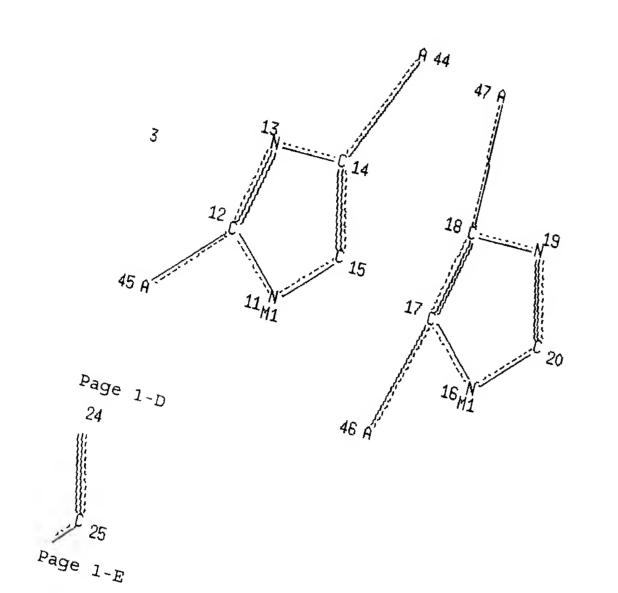
=> d 115 L15 HAS NO ANSWERS L15 STR

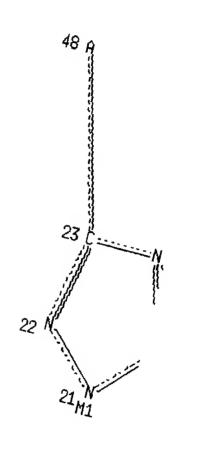


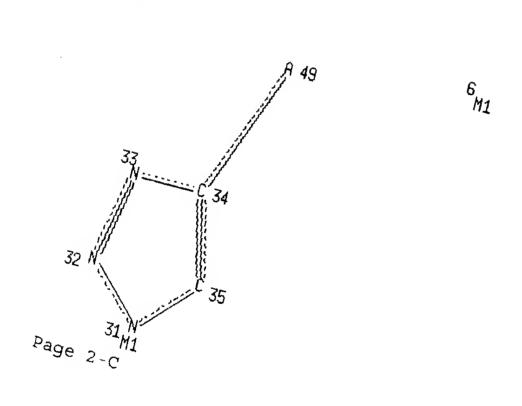
Page 1-A

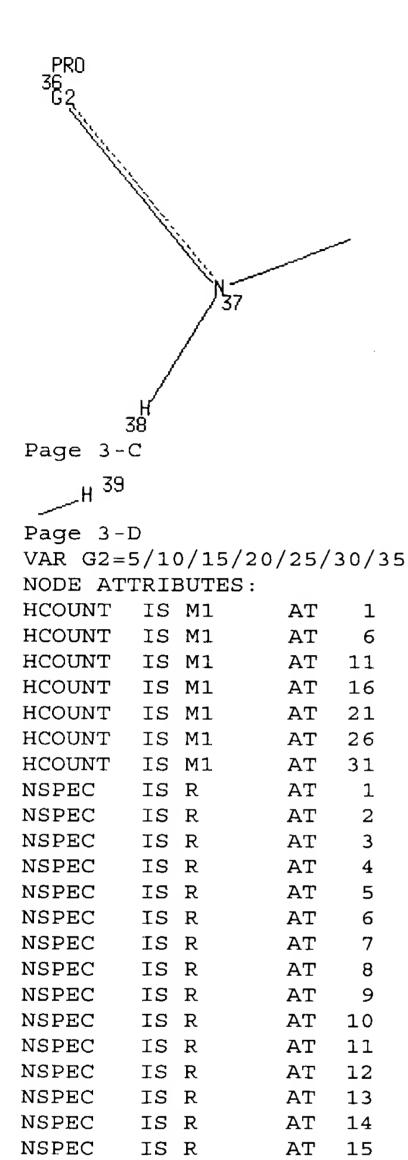












NSPEC

IS R

AT

16

17

18

19

20

21

22

23

24

25

26

27

28

29

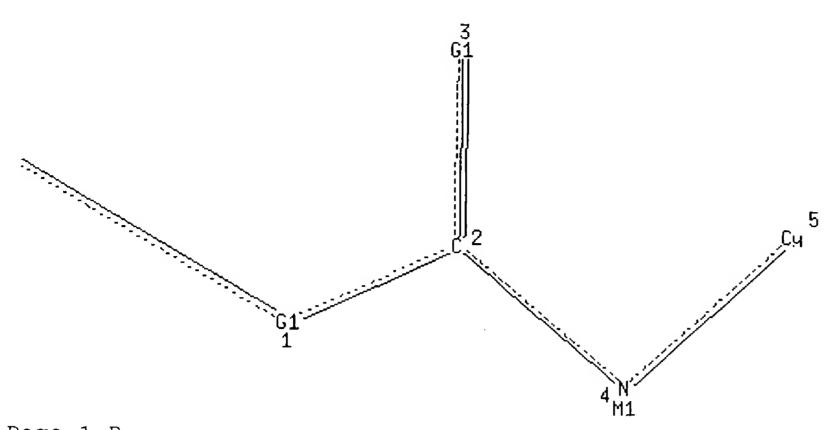
30

31

```
NSPEC
         IS R
                    AT 32
NSPEC
         IS R
                    \mathtt{AT}
                         33
NSPEC
         IS R
                    AT
                         34
NSPEC
         IS R
                    AT
                         35
NSPEC
         IS C
                    TA
                         36
NSPEC
         IS C
                    \mathtt{AT}
                         37
NSPEC
         IS C
                    AT
                         38
         IS C
NSPEC
                    AT
                         39
NSPEC
         IS RC
                    \mathsf{AT}
                         40
NSPEC
         IS RC
                    AT
                         41
NSPEC
         IS RC
                    \mathtt{AT}
                         42
NSPEC
         IS RC
                    AT
                         43
NSPEC
         IS RC
                    AT
                         44
NSPEC
         IS RC
                    AT
                         45
NSPEC
         IS RC
                    \mathtt{AT}
                         46
NSPEC
         IS RC
                    \mathtt{AT}
                         47
NSPEC
         IS RC
                    AT
                         48
         IS RC
NSPEC
                    AT
                         49
DEFAULT MLEVEL IS ATOM
MLEVEL
        IS CLASS
                    \mathtt{AT}
                         37 38 39 40 41 42 43 44 45 46 47 48 49
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS
                      49
STEREO ATTRIBUTES: NONE
=> s 115
SAMPLE SEARCH INITIATED 09:55:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 28473 TO ITERATE
  3.5% PROCESSED
                      1000 ITERATIONS
                                                                       8 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                           ONLINE
                                    **INCOMPLETE**
                           BATCH
                                    **COMPLETE**
PROJECTED ITERATIONS:
                                             579541
                               559379 TO
PROJECTED ANSWERS:
                                 3650 TO
                                               5460
L16
                8 SEA SSS SAM L15
=>
L17
         STRUCTURE UPLOADED
=> d 117
L17 HAS NO ANSWERS
L17
                  STR
07 S8
```

6 C.

Page 1-A



Page 1-B VAR G1=7/8NODE ATTRIBUTES: HCOUNT IS M1 AT NSPEC IS C ATNSPEC IS C ATNSPEC IS C ATNSPEC IS C ATNSPEC IS C 5 ATNSPEC IS RC ATDEFAULT MLEVEL IS ATOM MLEVEL IS CLASS ATDEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

=> s 117

SAMPLE SEARCH INITIATED 10:01:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 53469 TO ITERATE

1.9% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

EXCEEDS 1000000

PROJECTED ANSWERS:

EXCEEDS 143477

L18 50 SEA SSS SAM L17

```
=> e indanyl/cn
                   INDANTRIONE/CN
E1
                   INDANTRIONE HYDRATE/CN
E2
             0 --> INDANYL/CN
E3
                   INDANYL (4-(4-(PIPERIDINYL)BUT-1-YNYL)BENZYL)AMINE/CN
E4
             1
1
                   INDANYL CARBENICILLIN/CN
E5
                   INDANYL CARBENICILLIN SODIUM SALT/CN
E6
                   INDANYL MESYLATE/CN
E7
```

50 ANSWERS

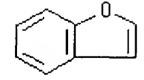
```
E8
             1
                   INDANYLIUM, 2-((3-ETHOXY-5-METHOXYINDEN-2-YL)METHYLENE)-1-HY
                   DROXY-6-METHOXY-/CN
E9
                   INDANYLPHENOL/CN
             1
E10
             1
                   INDAPAMIDE/CN
E11
             1
                   INDAQUASSIN A/CN
E12
             1
                   INDAQUASSIN B/CN
=> s e7
L19
             1 "INDANYL MESYLATE"/CN
=> d 119
L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
     777-72-0 REGISTRY
RN
     1H-Inden-2-ol, 2,3-dihydro-, methanesulfonate (9CI)
CN
                                                           (CA INDEX NAME)
OTHER CA INDEX NAMES:
     2-Indanol, methanesulfonate (7CI, 8CI)
OTHER NAMES:
     2-Indanyl methanesulfonate
CN
     Indanyl mesylate
CN
CN
     NSC 80565
FS
     3D CONCORD
MF
     C10 H12 O3 S
                  BEILSTEIN*, CA, CAOLD, CAPLUS, PS, TOXCENTER, USPATFULL
LC
     STN Files:
         (*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
       Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.P
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent);
       NORL (No role in record)
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)
10 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> e benzofuran/cn
E1
             1
                   BENZOFUR GG/CN
                   BENZOFUR P/CN
E2
             1
E3
             1 --> BENZOFURAN/CN
E4
             1
                   BENZOFURAN POLYMER/CN
                   BENZOFURAN RADICAL CATION/CN
E5
                   BENZOFURAN, ((2,4-DICHLOROPHENOXY) METHYL) -/CN
E6
             1
                   BENZOFURAN, (2-PROPENYL)-/CN
E7
             1
E8
             1
                   BENZOFURAN, 2 (OR 3) -METHYL-/CN
                   BENZOFURAN, 2,-BIS((P-AMINOPHENYL)ACETYL)-6-METHOXY-/CN
E9
             1
                   BENZOFURAN, 2,2',2'',2'''-(3,6-DIMETHYL-1,2,4,5-BENZENETETRA
E10
             1
                   YL) TETRAKIS-/CN
                   BENZOFURAN, 2,2',2'',2'''-(9,9'-SPIROBI(9H-FLUOREN)-2,2',7,7
E11
             1
                    '-TETRAYL) TETRAKIS-/CN
E12
             1
                   BENZOFURAN, 2,2',2'',2'''- (METHANETETRAYLTETRA-4,1-PHENYLENE
                   )TETRAKIS-/CN
```

```
=> s e3
L20
             1 BENZOFURAN/CN
=> d 120
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
L20
RN
     271-89-6 REGISTRY
     Benzofuran (6CI, 8CI, 9CI) (CA INDEX NAME)
CN
OTHER NAMES:
CN
     1-Oxindene
CN
     2,3-Benzofuran
CN
     AT 33852
CN
     Benzofurfuran
CN
     Benzo[b] furan
     Coumarone
CN
CN
     NSC 1255
CN
     R 7204
FS
     3D CONCORD
MF
     C8 H6 O
CI
     COM, RPS
                  AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS,
LC
     STN Files:
       BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, ENCOMPLIT,
       ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB,
       IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA,
       PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2,
       USPATFULL, VTB
         (*File contains numerically searchable property data)
     Other Sources:
                      DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA Caplus document type: Book; Conference; Dissertation; Journal; Patent;
       Preprint; Report
       Roles from patents: ANST (Analytical study); BIOL (Biological study);
RL.P
       FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses); NORL (No role in record)
      Roles for non-specific derivatives from patents: ANST (Analytical
       study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation);
       PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES
       (Uses)
      Roles from non-patents: ANST (Analytical study); BIOL (Biological
RL.NP
       study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical
       study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC
       (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);
       PRP (Properties); RACT (Reactant or reagent); USES (Uses)
```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1993 REFERENCES IN FILE CA (1907 TO DATE)
263 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1993 REFERENCES IN FILE CAPLUS (1907 TO DATE) 59 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

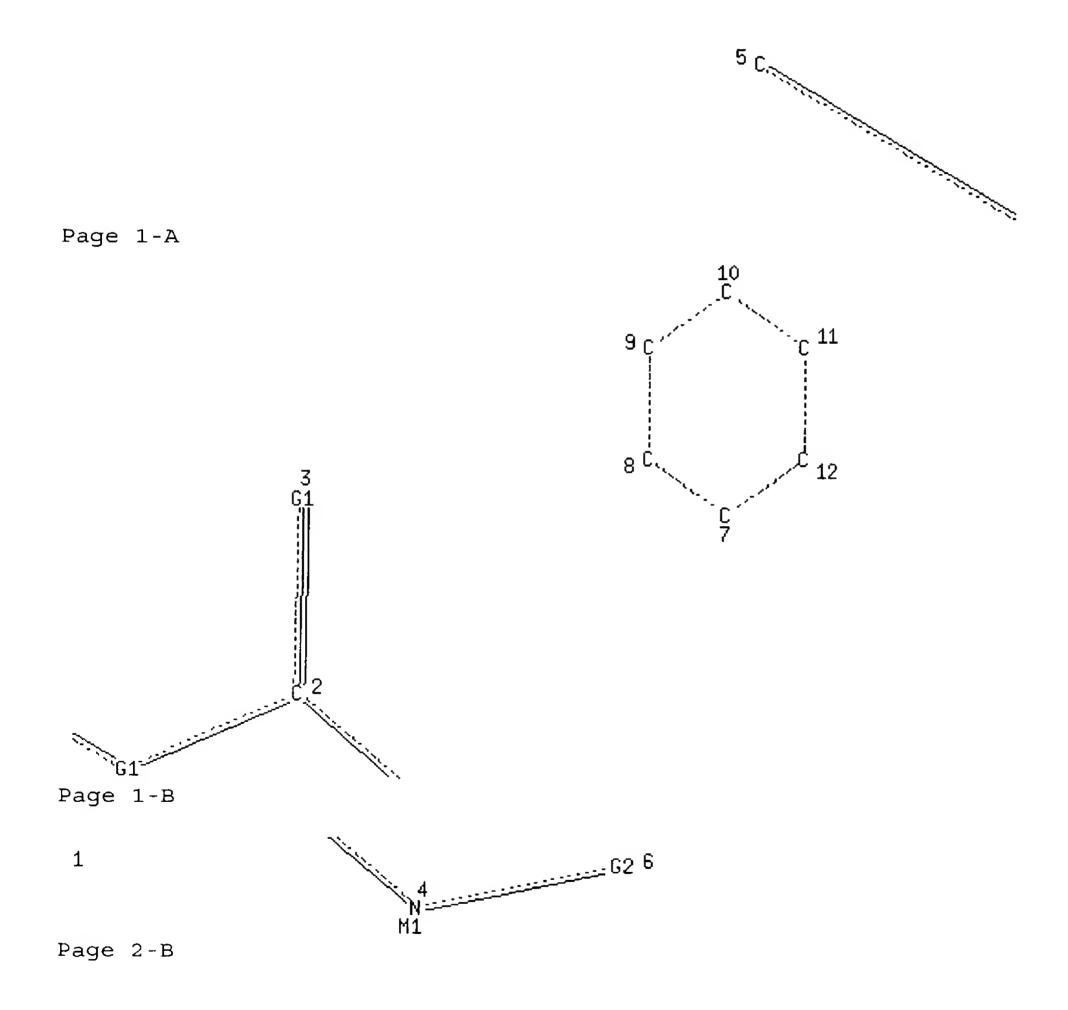
```
=> e indenyl/cn
E1
                    INDENOPYRENE, METHYL-/CN
E2
             1
                    INDENOPYRENONE/CN
             1 --> INDENYL/CN
E3
\mathbf{E4}
             1
                    INDENYL ANION/CN
E5
             1
                    INDENYL POTASSIUM/CN
E6
             1
                    INDENYL ZIRCONIUM TRIS (DIETHYLCARBAMATE) / CN
E7
             1
                    INDENYL ZIRCONIUM TRIS (TRIMETHYLACETATE) / CN
                    INDENYL (TRI (TERT-BUTYL) PHOSPHINIMIDO) TITANIUM DICHLORIDE/CN
E8
             1
             1
E9
                    INDENYL, 1,2,3,4,5,6,7-HEPTACHLORO-/CN
E10
             1
                    INDENYL, 1-DIOXY-/CN
E11
             1
                    INDENYL, 2-METHYL-/CN
E12
             1
                    INDENYL, 5-HYDROXY-/CN
=> s e3
L21
             1 INDENYL/CN
=> d 121
L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN
     71551-80-9 REGISTRY
CN
     Indenyl (7CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN
     Inden-2-yl
DR
     2143-54-6, 117988-54-2
MF
     C9 H7
CI
     MAN
LC
     STN Files:
                  BIOSIS, CA, CAOLD, CAPLUS, TOXCENTER
DT.CA CAplus document type: Dissertation; Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents:
       (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or
       reagent)
 STRUCTURE DIAGRAM IS NOT AVAILABLE
              24 REFERENCES IN FILE CA (1907 TO DATE)
               4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
              24 REFERENCES IN FILE CAPLUS (1907 TO DATE)
               2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
=>
L22
        STRUCTURE UPLOADED
```

=> d 122

L22

L22 HAS NO ANSWERS

STR



```
15
             18
 14
Page 3-B
  20
  21
Page 3-C
VAR G1=23/24
VAR G2 = 7/20
NODE ATTRIBUTES:
HCOUNT
         IS M1
                    AT
                          4
NSPEC
         IS C
                    AT
                          1
NSPEC
         IS C
                    AT
                          2
NSPEC
         IS C
                    AT
                          3
NSPEC
         IS C
                    AT
                          4
NSPEC
         IS RC
                          5
                    AT
NSPEC
         IS C
                    AT
                          6
NSPEC
                          7
         IS R
                    AT
NSPEC
         IS R
                    AT
                          8
NSPEC
         IS R
                          9
                    AT
NSPEC
         IS R
                         10
                    AT
NSPEC
         IS R
                    AT
                         11
NSPEC
                         12
         IS R
                    AT
NSPEC
         IS R
                         13
                    AT
NSPEC
         IS R
                    AT
                         14
NSPEC
         IS R
                    AT
NSPEC
         IS R
                    AT 16
NSPEC
                    AT 17
         IS R
NSPEC
                    AT 18
        IS R
NSPEC
        IS R
                    \mathtt{AT}
                        19
NSPEC
        IS R
                    \mathtt{AT}
                        20
                    \mathtt{AT}
NSPEC
         IS R
                        21
NSPEC
                    AT 22
         IS R
DEFAULT MLEVEL IS ATOM
MLEVEL
       IS CLASS AT
                          2 4 5 23 24
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 24
STEREO ATTRIBUTES: NONE
```

=> s 122 SAMPLE SEARCH INITIATED 10:10:45 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 12830 TO ITERATE 7.8% PROCESSED 1000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 249817 TO 263383

PROJECTED ANSWERS: 62503 TO 69389

L23 50 SEA SSS SAM L22

=> s 122 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 10:10:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 259836 TO ITERATE

100.0% PROCESSED 259836 ITERATIONS

65845 ANSWERS

SEARCH TIME: 00.00.02

L24 65845 SEA SSS FUL L22

=> file hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 189.14 575.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE 0.00 -1.98

FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 124/rct

26409 L24

2633407 RCT/RL

L25 6528 L24/RCT

(L24 (L) RCT/RL)

```
=> d his
     (FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)
     FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004
     FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004
L1
                 STRUCTURE UPLOADED
L2
              0 S L1
L3
              0 S L1 FULL
L4
                STRUCTURE UPLOADED
L5
              0 S L4
L6
              3 S L4 FULL
     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
                STRUCTURE UPLOADED
L7
     FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
             50 S L7
L8
           1575 S L7 FULL
Ь9
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
L10
            225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                STRUCTURE UPLOADED
L12
             50 S L11
                STRUCTURE UPLOADED
L13
L14
             49 S L13
L15
                STRUCTURE UPLOADED
L16
              8 S L15
L17
                STRUCTURE UPLOADED
             50 S L17
L18
                E INDANYL/CN
L19
              1 S E7
                E BENZOFURAN/CN
L20
              1 S E3
                E INDENYL/CN
L21
              1 S E3
L22
                STRUCTURE UPLOADED
L23
             50 S L22
L24
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
           6528 S L24/RCT
L25
=> s 125 and 110
            21 L25 AND L10
L26
=> file reg
COST IN U.S. DOLLARS
                                                   SINCE FILE
                                                                   TOTAL
                                                        ENTRY
                                                                 SESSION
FULL ESTIMATED COST
                                                         9.44
                                                                  584.74
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                  SINCE FILE
                                                                   TOTAL
                                                        ENTRY
                                                                 SESSION
CA SUBSCRIBER PRICE
                                                         0.00
                                                                   -1.98
```

FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

L27 STRUCTURE UPLOADED

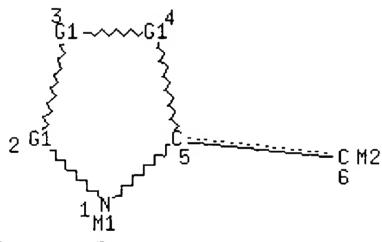
STR

=> d 127

L27 HAS NO ANSWERS

L27

C 7 N 8 Page 1-A



Page 1-B VAR G1=7/8

NODE ATTRIBUTES:

HCOUNT	IS	Ml	AT	1
HCOUNT	IS	M2	AT	6
NSPEC	IS	R	AT	1
NSPEC	IS	R	TA	2
NSPEC	IS	R	TA	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	C	AT	6
DEFAULT	MLE	EVEL IS	MOTA	
MLEVEL	IS	CLASS	TA	6

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

http://stnweb.cas.org/cgi-bin/sdcgi?SID=73665-0268560164-200&APP=stnweb&

=> s 127

SAMPLE SEARCH INITIATED 10:13:23 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 244417 TO ITERATE

1000 ITERATIONS 0.4% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH

PROJECTED ITERATIONS:

INCOMPLETE **EXCEEDS 1000000**

PROJECTED ANSWERS:

EXCEEDS 329523

50 SEA SSS SAM L27 L28

=> file hcaplus

TOTAL SINCE FILE COST IN U.S. DOLLARS SESSION ENTRY 585.16 0.42 FULL ESTIMATED COST

TOTAL SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SESSION ENTRY -1.980.00 CA SUBSCRIBER PRICE

FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

STRUCTURE UPLOADED L1

0 S L1 L2

0 S L1 FULL L3

STRUCTURE UPLOADED L4

```
L5
              0 S L4
L6
              3 S L4 FULL
     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
L7
                 STRUCTURE UPLOADED
     FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
L8
              50 S L7
L9
           1575 S L7 FULL
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
            225 S L9/PREP
L10
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                 STRUCTURE UPLOADED
L12
             50 S L11
                 STRUCTURE UPLOADED
L13
             49 S L13
L14
L15
                 STRUCTURE UPLOADED
L16
              8 S L15
L17
                 STRUCTURE UPLOADED
L18
             50 S L17
                E INDANYL/CN
L19
              1 S E7
                E BENZOFURAN/CN
L20
              1 S E3
                E INDENYL/CN
L21
              1 S E3
L22
                STRUCTURE UPLOADED
L23
             50 S L22
L24
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
           6528 S L24/RCT
L25
L26
             21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                 STRUCTURE UPLOADED
L28
              50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
=> s 126 and tan, z?/au
          1089 TAN, Z?/AU
L29
             0 L26 AND TAN, Z?/AU
=> s 126 and song, j?/au
          4843 SONG, J?/AU
             0 L26 AND SONG, J?/AU
L30
=> d 126, ibib abs hitstr, 1-21
     ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
          Citing
   Full
         References
   Text
ACCESSION NUMBER:
                          2004:60480
                                      HCAPLUS
DOCUMENT NUMBER:
                          140:111415
                          Preparation of imidazole derivatives as chymase
TITLE:
                          inhibitors
                          Kitano, Masafumi; Yamaguchi, Hiroki
INVENTOR(S):
```

PATENT ASSIGNEE(S):

Sumitomo Pharmaceuticals Co., Ltd., Japan

SOURCE:

PCT Int. Appl., 122 pp.

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

CODEN: PIXXD2

DANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.		KI	ND DATE				APPLICATION NO.					DATE				
											-						
WO 2004007464 A			Α	.1 20040122				WO 2003-JP8682					20030708				
W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,	
	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	PG,	
	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,	TR,	
	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,	
	KZ,	MD,	RU,	ТJ													
RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	BG,	
	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	
	NL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	
	GW,	ML,	MR,	NE,	SN,	TD,	TG										
PRIORITY APP	LN.	INFO	. :				· ·	JP 2	002-2	2017	39	Α	2002	0710			
OTHER SOURCE	(S):			MARPAT 140:111415													
GI																	

The title compds. I [wherein X1 = (un)substituted alkylene; X2 and Q = independently a single bond or (un)substituted alkylene; Y1 = (hetero)cyclylene; Y2 = (hetero)cyclyl; M = (un)substituted CO2H, SO3H, CONH2, SO2NH2, -NHSO2H, or tetrazolyl, etc.; R1 and R2 = independently (hetero)cyclyl, H, halo, NO2, CN, CO2H, (un)substituted alkyl, alkenyl, alkynyl, alkoxycarbonyl, acyl, OH, NH2, CONH2, SO2NH2, SH, SOH, or SO2H, etc.] or prodrugs, or pharmaceutically acceptable salts thereof are prepd. For example, the compd. II was prepd. in a multi-step synthesis. II showed inhibitory activity with IC50 of 0.026 μ M against human chymase. I have chymase inhibitory activity, and are useful as a therapeutic agent for hypertension, cardiac failure, etc. (no data).

IT 647850-05-3P 647850-07-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of imidazole derivs. as chymase inhibitors)

RN 647850-05-3 HCAPLUS

CN

Benzoic acid, 2-[[[[1-(1-naphthalenylmethyl)-1H-imidazol-2-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 647850-07-5 HCAPLUS

CN Benzoic acid, 2-[[[methyl[1-(1-naphthalenylmethyl)-1H-imidazol-2-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

IT 259537-23-0P 439142-85-5P 647850-99-5P

647851-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of imidazole derivs. as chymase inhibitors)

RN 259537-23-0 HCAPLUS

CN Benzoic acid, 2-[(phenoxycarbonyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 439142-85-5 HCAPLUS

CN Carbamic acid, [2-(4-morpholinylcarbonyl)phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 647850-99-5 HCAPLUS

CN Morpholine, 4-[2-[[[1-(1-naphthalenylmethyl)-1H-imidazol-2-yl]amino]carbonyl]amino]benzoyl]- (9CI) (CA INDEX NAME)

647851-03-4 HCAPLUS RN

Benzoic acid, 2-[[[methyl[1-(1-naphthalenylmethyl)-1H-imidazol-2-CNyl]amino]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

COPYRIGHT 2004 ACS on STN ANSWER 2 OF 21 HCAPLUS L26

8

Citing Full References Text ACCESSION NUMBER:

HCAPLUS 2004:41269

140:77038 DOCUMENT NUMBER:

Preparation of 3-[heteroarylmethoxy]pyridines and TITLE:

their analogues as p38 map kinase inhibitors

Murray, Christopher William; Hartshorn, Michael John; INVENTOR(S):

Frederickson, Martyn; Congreve, Miles Stuart; Padova, Alessandro; Woodhead, Steven John; Gill, Adrian Liam;

Woodhead, Andrew James

Astex Technology Limited, UK PATENT ASSIGNEE(S):

PCT Int. Appl., 134 pp. SOURCE:

CODEN: PIXXD2

Patent DOCUMENT TYPE:

English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	К	IND	DATE			APPLICATION NO. DATE								
WO 2004004720	2004004720 A1 20040115					WO 2003-GB2864 20030703								
W: AE. A	- AG. AL	. AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
CO. (CR, CU	CZ	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
GM. F	iR, HU	, ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
LS. I	LT. LU	, LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
PG. I	PH. PL	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,
TR,	rr, rz	, UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,

```
KG, KZ, MD, RU
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
             NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
             GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:
                                        GB 2002-15383
                                                            20020703
                                        US 2002-393121P
                                                            20020703
                                        GB 2002-26149
                                                         A 20021108
OTHER SOURCE(S):
                         MARPAT 140:77038
GI
     Title compds. I [X=Y = CR2=CR3, CR2=N; R1 = H, halo, amino, etc.; R2-3 =
AB
    H, alkyl, aryl, etc.; R4 = carboaryl, heteroaryl; R5 = halo, amino,
     carboxamido, etc.] are prepd. For instance, 2-amino-3-benzyloxypyridine
     is prepd. by alkylation of 2-amino-3-hydroxypyridine with benzyl chloride.
    A related example, 2-amino-3-[2-phenylbenzyloxy]pyridine has IC50 <
     10μM for p38 map kinase. I are useful in the treatment of diseases
     ameliorated by inhibiting p38 MAP kinase.
IT 642084-55-7P, 2-[2-Fluoro-5-[[[[1-(tert-butyl)-3-phenylpyrazol-5-
    yl]amino]carbonyl]amino]benzyloxy]pyrazine 642085-05-0P,
    N-(5-(tert-Butyl)-2-phenyl-2H-pyrazol-3-yl)-N'-[4-chloro-3-(((pyridin-3-
    yl)oxy)methyl)phenyl]urea 642085-37-8P, N-(5-tert-Butyl-2-phenyl-
    2H-pyrazol-3-yl)-N'-[4-fluoro-3-(((pyrazin-2-yl)oxy)methyl)phenyl]urea
    642085-49-2P, N-[5-tert-Butyl-2-(2,4-difluorophenyl)-2H-pyrazol-3-
    yl]-N'-[4-fluoro-3-(pyrazin-2-yloxymethyl)phenyl]urea 642085-50-5P
    , N-[5-tert-Butyl-2-(4-chlorophenyl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-
     (pyrazin-2-yloxymethyl)phenyl]urea 642085-51-6P,
    N-[5-(4-Chlorophenyl)-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-52-7P, N-(5-tert-Butyl-2-p-tolyl-
    2H-pyrazol-3-yl)-N'-[4-fluoro-3-(pyrazin-2-yloxymethyl)phenyl]urea
    642085-53-8P, N-[5-(4-Chlorophenyl)-2-(4-fluorophenyl)-2H-pyrazol-
    3-yl]-N'-[4-fluoro-3-(pyrazin-2-yloxymethyl)phenyl]urea
    642085-54-9P, N-(2,5-Diphenyl-2H-pyrazol-3-yl)-N'-[4-fluoro-3-
    (pyrazin-2-yloxymethyl)phenyl]urea 642085-56-1P,
    N-(2-Benzyl-5-tert-butyl-2H-pyrazol-3-yl)-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-57-2P, N-(2-(Benzothiazol-2-yl)-5-
    (tert-butyl)-2H-pyrazol-3-yl)-N'-[4-fluoro-3-(((pyrazin-2-
    yl)oxy)methyl)phenyl]urea 642085-58-3P, N-[5-tert-Butyl-2-(6-
    chloropyridazin-3-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-59-4P, N-[5-tert-Butyl-2-(2,6-
    dimethylpyrimidin-4-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-61-8P, N-(5-(tert-Butyl)-2-
    (pyridin-4-yl)-2H-pyrazol-3-yl)-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-62-9P, N-[2-(4-Fluorophenyl)-5-
    (tetrahydrofuran-2-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-63-0P, N-[5-(tert-Butyl)-2-(4-
    (methanesulfonyl)phenyl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-64-1P, N-[2-(4-tert-Butylphenyl)-
    5-cyclopropyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyl]urea 642085-65-2P, N-[2-(4-Fluorophenyl)-5-
    (tetrahydropyran-4-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
    yloxymethyl)phenyllurea
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
    (Therapeutic use); BIOL (Biological study); PREP (Preparation);
```

USES (Uses)

(prepn. of 3-[heteroarylmethoxy]pyridines and their analogs as p38 map kinase inhibitors for treatment of arthritis)

RN 642084-55-7 HCAPLUS

Urea, N-[1-(1,1-dimethylethyl)-3-phenyl-1H-pyrazol-5-yl]-N'-[4-fluoro-3[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN

CN

642085-05-0 HCAPLUS

CN Urea, N-[4-chloro-3-[(3-pyridinyloxy)methyl]phenyl]-N'-[3-(1,1-dimethylethyl)-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu´

RN 642085-37-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN <u>642085-49-2</u> HCAPLUS

Urea, N-[1-(2,4-difluorophenyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-50-5 HCAPLUS

CN Urea, N-[1-(4-chlorophenyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 642085-51-6 HCAPLUS

CN Urea, N-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-52-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 642085-53-8 HCAPLUS

CN Urea, N-[3-(4-chlorophenyl)-1-(4-fluorophenyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN642085-54-9 HCAPLUS

Urea, N-(1,3-diphenyl-1H-pyrazol-5-yl)-N'-[4-fluoro-3-CN[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

642085-56-1 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(phenylmethyl)-1H-pyrazol-5-yl]-N'-[4-CNfluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN642085-57-2 HCAPLUS

Urea, N-[1-(2-benzothiazolyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-CNfluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

642085-58-3 HCAPLUS RN

Urea, N-[1-(6-chloro-3-pyridazinyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-CN

N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-59-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2,6-dimethyl-4-pyrimidinyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ N & & \\ NH & -C - NH & \\ & & \\$$

RN <u>642085-61-8</u> HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-pyridinyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 642085-62-9 HCAPLUS

Urea, N-[1-(4-fluorophenyl)-3-(tetrahydro-2-furanyl)-1H-pyrazol-5-yl]-N'[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-63-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-[4-(methylsulfonyl)phenyl]-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-64-1 HCAPLUS

Urea, N-[3-cyclopropyl-1-[4-(1,1-dimethylethyl)phenyl]-1H-pyrazol-5-yl]-N'[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN <u>642085-65-2</u> HCAPLUS

CN Urea, N-[1-(4-fluorophenyl)-3-(tetrahydro-2H-pyran-4-yl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

IT 642085-13-0P, (4-Fluoro-3-hydroxymethylphenyl)carbamic acid

tert-butyl ester 642085-14-1P, [4-Fluoro-3-(((pyrazin-2-

yl)oxy)methyl)phenyl]carbamic acid tert-butyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of 3-[heteroarylmethoxy]pyridines and their analogs as p38 map kinase inhibitors for treatment of arthritis)

RN 642085-13-0 HCAPLUS

Carbamic acid, [4-fluoro-3-(hydroxymethyl)phenyl]-, 1,1-dimethylethyl CNester (9CI) (CA INDEX NAME)

RN642085-14-1 HCAPLUS

Carbamic acid, [4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]-, CN1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing Full References Text

ACCESSION NUMBER: 2003:892762 HCAPLUS

DOCUMENT NUMBER: 139:395938

Preparation of ureas as positive allosteric modulators TITLE:

of the nicotinic acetylcholine receptor

Piotrowski, David W.; Rogers, Bruce N.; McWhorter, INVENTOR(S):

William W., Jr.; Walker, Daniel P.; Corbett, Jeffrey

W.; Groppi, Vincent E., Jr.; Rudmann, Daniel G.

Pharmacia & Upjohn Company, USA PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 159 pp.

CODEN: PIXXD2

Patent DOCUMENT TYPE: English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLI	CATION NO. I	PATE								
	 -											
WO 2003093250	A2 20031	113 <u>WO 20</u>	WO 2003-US11493 20030428									
W: AE, AG,	AL, AM, AT,	AU, AZ, BA, BB,	BG, BR, BY,	BZ, CA, CH, CN,								
CO, CR,	CU, CZ, DE, I	DK, DM, DZ, EC,	EE, ES, FI,	GB, GD, GE, GH,								
GM, HR,	HU, ID, IL,	IN, IS, JP, KE,	KG, KP, KR,	KZ, LC, LK, LR,								
LS, LT,	LU, LV, MA, I	MD, MG, MK, MN,	MW, MX, MZ,	NO, NZ, OM, PH,								
PL, PT,	RO, RU, SC, S	SD, SE, SG, SK,	SL, TJ, TM,	TN, TR, TT, TZ,								
UA, UG,	US, UZ, VC,	VN, YU, ZA, ZM,	ZW, AM, AZ,	BY, KG, KZ, MD,								
RU, TJ,	TM	•										
RW: GH, GM,	KE, LS, MW, N	MZ, SD, SL, SZ,	TZ, UG, ZM,	ZW, AT, BE, BG,								
CH, CY,	CZ, DE, DK, I	EE, ES, FI, FR,	GB, GR, HU,	IE, IT, LU, MC,								
NI. PT.	RO. SE. ST. S	SK TR BF BJ	CF. CG. CT.	CM. GA. GN. GO.								

GW, ML, MR, NE, SN, TD, TG

<u>US 2003236287</u> A1 20031225 <u>US 2003-423062</u> 20030425 PRIORITY APPLN. INFO.: <u>US 2002-377364P</u> P 20020503 US 2003-456941P P 20030324

OTHER SOURCE(S): MARPAT 139:395938

AB ANHCXNHB [X = 0, S; A = (un)substituted Ph, 6-membered N heteroaryl; B = (un)substituted 5-6-membered heteroaryl] were prepd. to treat diseases or conditions in which the α 7 nAChR is known to be involved (no data). Thus, 2,4-Me(MeO)C6H3NH2 was treated with 3-F3CC6H4CNO to give 2,4-Me(MeO)C6H3NHCONHC6H4CF3-3.

IT 553661-25-9P 625120-00-5P 625120-03-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of ureas as pos. allosteric modulators of the nicotinic acetylcholine receptor)

RN 553661-25-9 HCAPLUS

CN Carbamic acid, [3-(trifluoromethoxy)phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 625120-00-5 HCAPLUS

CN Carbamic acid, [4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylphenyl], phenyl ester (9CI) (CA INDEX NAME)

RN 625120-03-8 HCAPLUS

CN Carbamic acid, (5-chloro-2,4-dimethoxyphenyl)-, phenyl ester (9CI) (CA INDEX NAME)

IT 625117-68-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of ureas as pos. allosteric modulators of the nicotinic acetylcholine receptor)

RN 625117-68-2 HCAPLUS

CN Urea, N-(5-chloro-2,4-dimethoxyphenyl)-N'-1H-imidazol-2-yl- (9CI) (CA INDEX NAME)

L26 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

2003:508521 HCAPLUS

DOCUMENT NUMBER:

OCUMENT NUMBER: 13

139:86541

TITLE:

N-containing heterocycle stable free radicals and

rubber compositions containing them

INVENTOR(S):

Tomono, Keisuke; Miyashita, Naoshi; Shimada, Atsushi

Yokohama Rubber Co., Ltd., Japan

PATENT ASSIGNEE(S): SOURCE:

Jpn. Kokai Tokkyo Koho, 7 pp. CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE

JP 2003183276
APPLICATION NO. DATE

JP 2003183276
APPLN. INFO.:

JP 2001-380398
20011213

OTHER SOURCE(S):

MARPAT 139:86541

GI

$$\begin{array}{c} \text{Me Me} \\ \text{Me} \\ \text{Me} \end{array} \begin{array}{c} \text{NH} - \text{CO} - \text{O} \\ \text{NH} - \text{CO} - \text{O} \\ \text{NH} \end{array}$$

The radicals, which are stable at room temp. in the presence of O, have N-contg. heterocycles and ≥1 hydrogen bond-formable bonds chosen from (thio)urethane, (thio)urea, (thio)amide, (thio)ester, and ether. Thus, a test piece comprising vulcanized product of a compn. comprising RSS 1 (natural rubber) 100, I (manufd. from 2,4-TDI, 4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl, and 3-hydroxy-1,2,4-triazole) 0.1, HAF Shoblack N 339 (carbon black) 50, ZnO 3, sulfur 2, and other additives showed tan 0.1138 at 100°.

IT 552885-92-4P

RL: IMF (Industrial manufacture); MOA (Modifier or additive use);

PREP (Preparation); USES (Uses)

(N-contg. heterocycle stable free radicals as heat-stabilizers for rubber compns. with good vibration damping property)

RN 552885-92-4 HCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[[[2(or 4)-methyl-5-[[(1H-1,2,4-triazol-3-ylamino)carbonyl]amino]phenyl]amino]carbonyl]oxy]- (9CI) (CA INDEX NAME)

D1-Me

IT 376590-90-8P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP

(Preparation); RACT (Reactant or reagent)

(N-contg. heterocycle stable free radicals as heat-stabilizers for rubber compns. with good vibration damping property)

RN 376590-90-8 HCAPLUS

CN 1-Piperidinyloxy, 4-[[[[3(or 5)-isocyanato-4(or 2)-

methylphenyl]amino]carbonyl]oxy]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

D1-Me

L26 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

2002:428885 HCAPLUS

DOCUMENT NUMBER: 137:6179

TITLE: Preparation of benzimidazoles as TIE-2 and/or VEGFR2

inhibitors

INVENTOR(S): Cheung, Mui; Harris, Philip Anthony; Hasegawa,

Masaichi; Ida, Satoru; Kano, Kazuya; Nishigaki,

Naohiko; Sato, Hideyuki; Veal, James Martin; Washio,

Yoshiaki; West, Rob I.

PATENT ASSIGNEE(S): Glaxo Group Limited, UK; Glaxosmithkline K.K.

SOURCE: PCT Int. Appl., 217 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLIC	APPLICATION NO. DATE							
WO 2002044156	A2 20020606	WO 200	01-US44553	20011128						
WO 2002044156	A3 20021017									
W: AE, AG,	AL, AM, AT, AU,	AZ, BA, BB,	BG, BR, BY,	BZ, CA,	CH, CN,					
CO, CR,	CU, CZ, DE, DK,	DM, DZ, EC,	EE, ES, FI,	GB, GD,	GE, GH,					
GM, HR,	HU, ID, IL, IN,	IS, JP, KE,	KG, KP, KR,	KZ, LC,	LK, LR,					
LS, LT,	LU, LV, MA, MD,	MG, MK, MN,	MW, MX, MZ,	NO, NZ,	OM, PH,					
PL, PT,	RO, RU, SD, SE,	SG, SI, SK,	SL, TJ, TM,	TR, TT,	TZ, UA,					
UG, US,	UZ, VN, YU, ZA,	ZM, ZW, AM,	AZ, BY, KG,	KZ, MD,	RU, TJ, TM					
RW: GH, GM,	KE, LS, MW, MZ,	SD, SL, SZ,	TZ, UG, ZM,	ZW, AT,	BE, CH,					

CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2002-32439 20011128 AU 2002032439 20020611 **A**5 **A2** EP 2001-991963 20011128 20030910 EP 1341771 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR JP 2002-546526 20011128 JP 2004517080 T220040610 US 2004082583 **A**1 20040429 US 2003-433128 20031112 PRIORITY APPLN. INFO.: US 2000-253868P P 20001129 US 2001-310939P P 20010808 WO 2001-US44553 20011128

OTHER SOURCE(S): GΙ

MARPAT 137:6179

$$\begin{array}{c|c} Z & X & D & M-Q \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

The title compds. [I; E = (un) substituted aryl, heteroaryl; A = aryl, ABheteroaryl, heterocyclyl; X = S, O, SO2, SO, CH2, CHOH, CO; Z = O, S; p = 0-1; q = 0-1; D = CH, T = CR8, M = C and Q = NT7p, wherein p = 0 and q = 01; or D = CH, T = CR8, M = C and Q = NR7p, wherein p = 1 and q = 0, or D = 1CH, T = CR8, M = C and Q = S or O, wherein q = 0; or D = N, T = CR8, M = Cand Q = NR7p, wherein either p or q = 0 and the other = 1; or D = CH, T =N, M = C and Q = NR7p, wherein either p or q = 0 and the other = 1; or D = 0CH, T = CR8, M = N and Q = CH, wherein q = 0; R1 = alkyl, haloalkyl, aryl, etc.; R2 = H, alkyl, aryl, etc.; R3 = alkylene or alkylene substituted by oxo, and is linked together with N atom to which it is attached and to one of the benzimidazole N atoms to form a heterocyclic compd. fused to the benzimidazole; R7 = H, alkyl, etc.; R8 = H, halo] and their salts, useful in the treatment of hyperproliferative diseases, were prepd. Thus, reacting Me [5-(4-aminophenoxy)-1H-benzimidazol-2-yl]carbamate (prepn. given) with 3-chlorophenyl isocyanate in THF afforded 69% II which showed pIC50 of > 7.0 in TIE-2 and VEGFR2 enzyme assays.

ΙI

IT 433225-52-6P 433225-66-2P 433225-79-7P

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors)

433225-52-6 HCAPLUS RN

Acetamide, N-[5-[4-[[[5-(4-morpholinyl)-1H-1,2,4-triazol-3-CNyl]amino]carbonyl]amino]phenoxy]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 433225-66-2 HCAPLUS

CN Acetamide, 2-(2-methoxyethoxy)-N-[5-[4-[[[5-(4-morpholinyl)-1H-1,2,4-triazol-3-yl]amino]carbonyl]amino]phenoxy]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-B

- CH 2- CH 2- OMe

RN 433225-79-7 HCAPLUS

CN 2-Furancarboxamide, N-[5-[4-[[[5-(4-morpholinyl)-1H-1,2,4-triazol-3-yl]amino]carbonyl]amino]phenoxy]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

IT 433225-36-6P 433225-37-7P 433225-38-8P

433225-86-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors)

RN 433225-36-6 HCAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[[2-[[[2-fluoro-5-(trifluoromethyl)phenyl]amino]-1H-benzimidazol-5-yl]oxy]phenyl]- (9CI) (CA INDEX NAME)

RN 433225-37-7 HCAPLUS

Urea, N-[4-[[2-[[(4-chlorophenyl)amino]carbonyl]amino]-1H-benzimidazol-5-yl]oxy]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX

NAME)

RN 433225-38-8 HCAPLUS

Urea, N-[4-[[2-[[[4-(dimethylamino)phenyl]amino]carbonyl]amino]-1H-benzimidazol-5-yl]oxy]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

RN 433225-86-6 HCAPLUS

Urea, N-[4-[[2-[[[(2,3-dimethylphenyl)amino]carbonyl]amino]-1H-benzimidazol-5-yl]oxy]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

IT 54840-15-2, 4-(tert-Butoxycarbonyl)aminophenol 433226-40-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors)

RN 54840-15-2 HCAPLUS

CN Carbamic acid, (4-hydroxyphenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 433226-40-5 HCAPLUS

CN Carbamic acid, [6-[4-[[(1,1-dimethylethoxy)carbonyl]amino]phenoxy]-1H-imidazo[4,5-b]pyridin-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

$$t-BuO - C-NH$$

$$0$$

$$NH - C-OMe$$

IT 433226-08-5P, 2-Nitro-5-(4-(tert-butoxycarbonylamino)phenoxy)pyrid in-3-ylamine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors)

433226-08-5 HCAPLUS RN

Carbamic acid, [4-[(5-amino-6-nitro-3-pyridinyl)oxy]phenyl]-, CN1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 6 OF 21 L26HCAPLUS COPYRIGHT 2004 ACS on STN

136:340689

Citing Full References Text

ACCESSION NUMBER:

2002:314913 HCAPLUS

DOCUMENT NUMBER:

TITLE:

INVENTOR(S):

Preparation of urea derivatives containing nitrogenous

aromatic ring compounds as inhibitors of angiogenesis Funahashi, Yasuhiro; Tsuruoka, Akihiko; Matsukura,

Masayuki; Haneda, Toru; Fukuda, Yoshio; Kamata, Junichi; Takahashi, Keiko; Matsushima, Tomohiro; Miyazaki, Kazuki; Nomoto, Kenichi; Watanabe, Tatsuo; Obaishi, Hiroshi; Yamaguchi, Atsumi; Suzuki, Sachi; Nakamura, Katsuji; Mimura, Fusayo; Yamamoto, Yuji;

Matsui, Junji; Matsui, Kenji; Yoshiba, Takako; Suzuki,

Yasuyuki; Arimoto, Itaru Eisai Co., Ltd., Japan PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 699 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.		KI	ND :	D DATE APPLICATION N						ο.	DATE					
 -			- -														
WO 2002	0328	72	A	1 .	2002	0425	5 WO 2001-JP922					1	20011019				
WO 2002	0328	72	C	1 :	2002	0926											
W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
													NO,				
	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	
	US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM		
RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	
	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
													SN,				
AU 2001	0959	<u>86</u>	A ⁵	5 3	2002	0429		Al	J 200	01-9	5986		2001	1019			

EP 1415987 A1 20040506 EP 2001-976786 20011019 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR NO 2003001731 Α 20030619 NO 2003-1731 20030414 US 2004053908 A1 20040318 US 2003-420466 20030418 PRIORITY APPLN. INFO.: JP 2000-320420 A 20001020 JP 2000-386195 A 20001220 JP 2001-46685 A 20010222 W 20011019 WO 2001-JP9221 OTHER SOURCE(S): MARPAT 136:340689 GI

AΒ N-aryl or N-heteroarylurea derivs. represented by the general formula Ag-Xg-Yg-Tg1 or salts thereof, or hydrates of both [wherein Ag = (un) substituted C6-14 aryl or 5- to 14-membered heterocyclic group; Xg = single bond, O, S, C1-6 alkylene, SO, SO2, (un) substituted NH; Yq = (un) substituted C6-14 aryl, 5- to 14-membered heterocyclic group, C1-8 alkyl, C3-8 alicyclic hydrocarbyl, C6-14 aryl-C1-6 alkyl, 5- to 14-membered heteroaryl-C1-6 alkyl, (CH2)gSO2 (g = 1-8), (CH2) faCH: CH(CH2) fb (fa, fb = 0, 1, 2, 3), etc.; and Tg1 = a group of the general formula -Eg-CO-NRg1(Zg) or Q; wherein Eg = a single bond, (un) substituted NH; Rg1 = H, (un) substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 aliph. hydrocarbyl, etc.; Zg = C1-8 alkyl, C3-8 alicyclic hydrocarbyl, C6-14 aryl, etc.; Zg1, Zg2 = (a) a single bond, (b) C1-6 alkylene optionally having ≥ 1 atoms selected from O, S, and N in the middle or the terminus of the chain and optionally substituted with oxo, (c) (un) substituted C2-6 alkenyl] are prepd. These compds. are also inhibitors of vascular endothelial growth factor receptor kinase (VEGFR2 kinase) and are useful as antitumor agents against hemangioma, pancreatic cancer, stomach cancer, colon cancer, breast cancer, prostate cancer, lung cancer, brain tumor, leukemia, or ovarian cancer, as cancer metastasis inhibitors, and for the treatment of retina neovascularization, diabetic retinopathy, atherosclerosis, or inflammatory diseases such as osteoarthritis, rheumatoid arthritis, psoriasis, or delayed hypersensitivity. Thus, to soln. of 334 mg 4-[6-(4-benzyloxyphenyl)-7-(2trimethylsilylethoxymethyl) -7H-pyrrolo[2,3-d]pyrimidin-4-yloxy]-2chlorophenylamine in 4 mL DMF were added 0.066 mL pyridine and 0.102 mL Ph chlorocarbonate and stirred at room temp. for 2.5 h to give 330 mg N-[4-[6-(4-benzyloxyphenyl)-7-(2-trimethylsilylethoxymethyl)-7Hpyrrolo[2,3-d]pyrimidin-4-yloxy]-2-chlorophenyl]-N'-cyclopropylurea which (260 mg) was hydrogenolyzed over platinum oxide in ethanol overnight to give 160 mg N-[4-[6-(4-hydroxyphenyl)-7-(2-trimethylsilylethoxymethyl)-7Hpyrrolo[2,3-d]pyrimidin-4-yloxy]-2-chlorophenyl]-N'-cyclopropylurea (I). I showed IC50 of 0.02 nM for inhibiting the vascular endothelial growth factor (VEGF)-stimulated sandwich tube formation in vascular endothelial cell.

IT 417713-01-0P 417713-68-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

RN 417713-68-9 HCAPLUS

CN Urea, N-1H-benzimidazol-2-yl-N'-[4-[[6-cyano-7-(2-methoxyethoxy)-4-quinolinyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

IT 4930-03-4, Phenylcarbamic acid phenyl ester

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of urea derivs. contg. nitrogenous arom. ring compds. as angiogenesis inhibitors for prevention or treatment of diseases)

RN 4930-03-4 HCAPLUS

CN Carbamic acid, phenyl-, phenyl ester (9CI) (CA INDEX NAME)

RN 65141-04-0 HCAPLUS

CN Carbamic acid, (4-fluorophenyl)-, phenyl ester (9CI) (CA INDEX NAME)

RN 347151-53-5 HCAPLUS

CN Carbamic acid, [4-[(6,7-dimethoxy-4-quinolinyl)oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417721-09-6</u> HCAPLUS

CN Carbamic acid, [4-[[6-cyano-7-(2-methoxyethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN417721-10-9 HCAPLUS

Carbamic acid, [4-[[6-cyano-7-(2-methoxyethoxy)-4-quinolinyl]oxy]-2-CNfluorophenyl] -, phenyl ester (9CI) (CA INDEX NAME)

RN417721-11-0 HCAPLUS

Carbamic acid, [4-[(6-cyano-7-methoxy-4-quinolinyl)oxy]phenyl]-, phenyl CNester (9CI) (CA INDEX NAME)

RN417721-13-2 **HCAPLUS**

Carbamic acid, [3-(methylsulfonyl)phenyl]-, phenyl ester (9CI) CN(CA INDEX NAME)

$$Me = \begin{cases} 0 & \text{NH} = 0 \\ 0 & \text{OPh} \end{cases}$$

417721-32-5 RN**HCAPLUS** CN Carbamic acid, [4-[[6-cyano-7-(phenylmethoxy)-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417721-91-6 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[4-[3-chloro-4-[(phenoxycarbonyl)amino]phenoxy]-2-pyridinyl]amino]carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 417722-40-8 HCAPLUS

CN 6-Quinolinecarboxylic acid, 4-[3-chloro-4-[(phenoxycarbonyl)amino]phenoxy]-7-(2-methoxyethoxy)-, methyl ester (9CI) (CA INDEX NAME)

RN 417722-53-3 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-3-methylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{H}_2\text{N} - C \\ \text{O} \\ \text{PhO} - C - \text{NH} \\ \text{O} \\ \end{array}$$

RN 417722-83-9 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417722-87-3 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-(2-methoxyethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417722-91-9 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-(2-methoxyethoxy)-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

417722-95-3 HCAPLUS RN

Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-CNchlorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN417722-99-7 **HCAPLUS**

Carbamic acid, [4-[[6-(aminocarbonyl)-7-(phenylmethoxy)-4-quinolinyl]oxy]-CN2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN417723-05-8 HCAPLUS

Carbamic acid, [4-[[6-(aminocarbonyl)-7-(phenylmethoxy)-4-quinolinyl]oxy]-CN2-chlorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417723-09-2 HCAPLUS

CN 6-Quinolinecarboxylic acid, 4-[3-chloro-4-[(phenoxycarbonyl)amino]phenoxy]-7-methoxy-, methyl ester (9CI) (CA INDEX NAME)

RN <u>417723-58-1</u> HCAPLUS

CN Carbamic acid, [4-[[2-[(1-oxobutyl)amino]-4-pyridinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417723-70-7</u> HCAPLUS

CN Carbamic acid, [4-[[7-methoxy-6-[(methylamino)carbonyl]-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417723-73-0 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-methylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417723-76-3</u> HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-(trifluoromethyl)phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417723-78-5 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2,3-dimethylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417723-81-0 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2,5-dimethylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417724-07-3 HCAPLUS

CN Carbamic acid, [4-[[6-cyano-7-[(2R)-oxiranylmethoxy]-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 417724-17-5 HCAPLUS

Carbamic acid, [2-chloro-5-[[6-cyano-7-[(2R)-2-hydroxy-3-(1-pyrrolidinyl)propoxy]-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 417724-33-5 HCAPLUS

CN Carbamic acid, [4-[(6,7-dimethoxy-4-quinolinyl)oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417724-40-4</u> HCAPLUS

CN Carbamic acid, [4-[[6-cyano-7-[3-(1-piperidinyl)propoxy]-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417724-41-5 HCAPLUS

CN Carbamic acid, [2-chloro-4-[[6-cyano-7-(phenylmethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417724-46-0 HCAPLUS

CN Carbamic acid, [2-chloro-4-[[6-[(methylamino)carbonyl]-7-(phenylmethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417724-54-0 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[6-cyano-4-[3-fluoro-4-[(phenoxycarbonyl)amino]phenoxy]-7-quinolinyl]oxy]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 417724-59-5 HCAPLUS

CN 6-Quinolinecarboxylic acid, 4-[3-fluoro-4-[(phenoxycarbonyl)amino]phenoxy]-7-methoxy-, methyl ester (9CI) (CA INDEX NAME)

RN 417724-65-3 HCAPLUS

CN Carbamic acid, [4-[[6-cyano-7-(phenylmethoxy)-4-quinolinyl]oxy]-2,3-dimethylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417724-88-0 HCAPLUS

7-Piperidinecarboxylic acid, 4-[2-[[4-[3-chloro-4-[(phenoxycarbonyl)amino]phenoxy]-2-pyridinyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

17

Full Citing Text References

ACCESSION NUMBER: DOCUMENT NUMBER:

2001:468189 HCAPLUS

135:61321

TITLE:

Methods for the solid phase synthesis of combinatorial

libraries of benzimidazoles, benzoxazoles, benzothiazoles and derivatives for use as

peptidomimetics

INVENTOR(S):

Laborde, Edgardo; Matsumoto, Yukiharu

PATENT ASSIGNEE(S):

Telik, Inc., USA U.S., 18 pp.

SOURCE:

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLIC	CATION NO	Ο.	DATE
US 6251689	B1	20010626	US 199	99-313568	3_	19990514
US 2001024833	A1	20010927	US 200	1-775644	<u>1</u>	20010205
PRIORITY APPLN. INFO.	:		US 1998-8	35465P	P	19980514
			US 1999-3	313568	A1	19990514

OTHER SOURCE(S): CASREACT 135:61321

The present invention provides an efficient and versatile method for the synthesis and screening of combinatorial libraries of benzimidazoles, benzoxazoles, benzothiazoles, and derivs. thereof. Thus, resin-bound 4-carboxybenzaldehyde in DMA is treated with 1,2-phenylenediamine and TCNE to give 2-(4-carboxyphenyl)benzimidazole. In order to expedite the synthesis of large arrays of compds. possessing these core structures, a general methodol. for solid phase synthesis of these derivs. is provided. Arrays of benzimidazoles, benzoxazoles, benzothiazoles, and derivs. thereof useful as peptidomimetics and for the identification of agents having antifungal, antiviral, antimicrobial, anticoagulant, and antiulcer activity, or use in the treatment of inflammation, hypertension, cancer, and other conditions can be prepd. by this method.

IT 345958-22-7D, resin bound

RL: RCT (Reactant); RACT (Reactant or reagent)

(methods for the solid phase synthesis of combinatorial libraries of benzimidazoles, benzoxazoles, benzothiazoles and derivs. for use as peptidomimetics)

RN 345958-22-7 HCAPLUS

CN Benzoic acid, 3,4-bis[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

IT 345958-14-7P 345958-15-8P 345958-17-0P

RL: SPN (Synthetic preparation); **PREP (Preparation)**(methods for the solid phase synthesis of combinatorial libraries of benzimidazoles, benzoxazoles, benzothiazoles and derivs. for use as peptidomimetics)

RN 345958-14-7 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[(phenylamino)carbonyl]amino](9CI) (CA INDEX NAME)

RN 345958-15-8 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[[[3-(trifluoromethyl)phenyl]amino] carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 345958-17-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:666713 HCAPLUS

DOCUMENT NUMBER: 133:252426

TITLE: Preparation of aromatic heterocyclic ureas as

antiinflammatory agents

INVENTOR(S): Betageri, Rajashehar; Breitfelder, Steffen; Cirillo,

Pier F.; Gilmore, Thomas A.; Hickey, Eugene R.; Kirrane, Thomas M.; Moriak, Monica H.; Moss, Neil; Patel, Usha R.; Proudfoot, John R.; Regan, John R.;

Sharma, Rajiv; Sun, Sanxing; Swinamer, Alan D.;

Takahashi, Hidenori

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 282 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	DATE APPLICATION NO. DATE									
	-											
WO 2000055139	A2	20000921	WO 2000-US3865 2000021						0216			
WO 2000055139	A3	20010426										
W: AE, AU	BG, BR	, BY, CA,	CN,	CZ,	EE,	HR,	HU,	ID,	IL,	IN,	JP,	KR,
KZ, LT	LV, MX	, NO, NZ,	PL,	RO,	RU,	SG,	SI,	SK,	TR,	UA,	UZ,	VN,
YU, ZA												
RW: AT, BE	CH, CY	, DE, DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,
PT, SE												
EP 1165516	A2	20020102		E	P 200	00-9	0729	5	2000	0216		
R: AT, BE	CH, DE	. DK. ES.	FR.	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,

GI

The title compds. (I) [wherein Ar1 = (un) substituted pyrrole, pyrrolidine, pyrazole, imidazole, oxazole, thiazole, furan, or thiophene; Ar2 = (un) substituted Ph, (tetrahydro) naphthyl, (tetrahydro) quinoline, (tetrahydro) isoquinoline, benzimidazole, benzofuran, indanyl, indenyl, or indole; W = O or S; X = (un) substituted cycloalkyl, cycloalkenyl, Ph, furan, thiophene, pyrrole, imidazolyl, pyridine, pyrimidine, (dihydro) pyridinone, (dihydro) maleimide, piperidine, piperazine, or pyrazine; Y = a bond or (un) substituted satd. or unsatd. alkyl optionally interrupted by O, NH, S(O), SO2, or S; Z = (un) substituted Ph, pyridine, pyrimidine, pyridazine, imidazole, (tetrahydro) furan, thiophene, (tetrahydro) pyran, 1,3-dioxolanone, 1,3-dioxanone, 1,4-dioxane, (thio) morpholine (sulfoxide), piperidine, cyclohexanone, pentamethylene sulfoxide, etc.] were prepd. for the treatment of diseases or pathol.

ΙΙ

conditions involving inflammation, such as chronic inflammatory diseases. Thus, coupling 2-cyclohexenone with 4-bromo-1-naphthylamine in the presence of Pd(PPh3)2Cl2, DPPP, and NaHCO3 in DMF, followed by conversion of the amine to an isocyanate using ClCOCl and immediate addn. of 1-(4-methylphenyl)-3-tert-butyl-1H-pyrazol-5-amine, gave the urea II. In a cytokine prodn. inhibition assay, preferred compds. of the invention showed IC50 < 10 .mu.M against TNF-.alpha. in lipopolysaccharide stimulated THF cells.

IT 294851-78-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of arom. heterocyclic urea antiinflammatory agents by conversion of arylamines to isocyanates followed by addn. of heterocyclic amines)

RN 294851-78-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[3-oxo-1-cyclohexen-1-yl)-1-naphthalenyl]- (9CI) (CA INDEX NAME)

IT 294848-43-4P 294848-46-7P 294848-49-0P 294848-51-4P 294848-53-6P 294848-55-8P 294848-58-1P 294848-61-6P 294848-64-9P 294848-67-2P 294848-70-7P 294848-73-0P 294848-76-3P 294848-79-6P 294848-82-1P 294848-85-4P 294848-88-7P 294848-91-2P 294848-94-5P 294848-96-7P 294848-98-9P 294849-00-6P 294849-02-8P 294849-04-0P 294849-06-2P 294849-08-4P 294849-10-8P 294849-12-0P 294849-14-2P 294849-16-4P 294849-18-6P 294849-20-0P 294849-22-2P 294849-24-4P 294849-26-6P 294849-28-8P 294849-30-2P 294849-32-4P 294849-34-6P 294849-36-8P 294849-38-0P 294849-40-4P 294849-42-6P 294849-44-8P 294849-46-0P 294849-48-2P 294849-50-6P 294849-52-8P 294849-54-0P 294849-56-2P 294849-58-4P 294849-60-8P 294849-62-0P 294849-64-2P 294849-66-4P 294849-68-6P 294851-79-9P 294851-81-3P 294851-83-5P 294851-85-7P 294853-11-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of arom. heterocyclic urea antiinflammatory agents by conversion of arylamines to isocyanates followed by addn. of heterocyclic amines)

294848-43-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-LIU (1-4-morpholinylmethyl)) (CA INDEX NAME)

PAGE 1-A

RN

CN

PAGE 2-A

RN 294848-46-7 HCAPLUS
CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[
[4-[2-(4-morpholinyl)ethyl]phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

294848-49-0 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-□ CN[3-(4-morpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

294848-51-4 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-CN[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294848-53-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[5-(4-morpholinylmethyl)-2-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-55-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[5-(4-morpholinylmethyl)-2-furanyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294848-58-1 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-□
N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA
INDEX NAME)

PAGE 2-A

RN 294848-61-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[6-(4-\)morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-64-9 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[3-[[2-(2-pyridinyl)ethyl]amino]-1-cyclohexen-1-yl]-1-naphthalenyl](9CI) (CA INDEX NAME)

RN 294848-67-2 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[4-[4-[(3-pyridinylmethyl)amino]methyl]phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-70-7 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-UN'-[4-[4-(4-morpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294848-73-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(4-hydroxybutyl)amino]-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-76-3 HCAPLUS

CN Benzamide, 5-[3-(1,1-dimethylethyl)-5-[[[[4-[6-(4-morpholinylmethyl)-3-[] pyridinyl]-1-naphthalenyl]amino]carbonyl]amino]-1H-pyrazol-1-yl]-2-methyl-(9CI) (CA INDEX NAME)

PAGE 1-A

RN 294848-79-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- \square N'-[4-[4-[(3-hydroxy-1-piperidinyl)methyl]phenyl]-1-naphthalenyl]- (9CI)

(CA INDEX NAME)□

PAGE 1-A

RN 294848-82-1 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-□
N'-[4-[4-[(4-oxido-4-morpholinyl)methyl]phenyl]-1-naphthalenyl]- (9CI)
(CA INDEX NAME)□

PAGE 2-A

RN294848-85-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-□ CNN'-[4-[3-(4-morpholinylmethyl)-1-cyclohexen-1-yl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

294848-88-7 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-CNN'-[4-[3-hydroxy-4-[(tetrahydro-3-furanyl)methyl]phenyl]-1-naphthalenyl]-(CA INDEX NAME) (9CI)

PAGE 2-A

RN 294848-91-2 HCAPLUS

Urea, N-[4-[4-[[bis(2-methoxyethyl)amino]methyl]phenyl]-1-naphthalenyl]-N'-L [3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)L

RN 294848-94-5 HCAPLUS

Urea, N-[4-[6-(3-cyanopropoxy)-3-pyridinyl]-1-naphthalenyl]-N'-[3-(1,1dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 294848-96-7 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[4-(4-morpholinylmethyl)-1-piperidinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-98-9 HCAPLUS

Urea, N-[4-[4-[[bis(2-cyanoethyl)amino]methyl]phenyl]-1-naphthalenyl]-N'-L [3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-00-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[4-(2-furanylmethyl)-3-hydroxyphenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-02-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[4-(4-thiomorpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-04-0 HCAPLUS

ON 3-Piperidinecarboxamide, 1-[[4-[4-[[[[3-(1,1-dimethylethyl)-1-(6-methyl-3-[pyridinyl)-1H-pyrazol-5-yl]amino]carbonyl]amino]-1-[naphthalenyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-06-2 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[4-[(2-methyl-3-oxo-1-piperazinyl)methyl]phenyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-08-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]-□
N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA
INDEX NAME)

RN 294849-10-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-(4-hydroxybutoxy)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-12-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)[1,4'-bi-1H-pyrazol]-5-yl]-N'-[4-[6-(4- \sqcup morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-14-2 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-2H-thiopyran-4-yl)amino]-3-pyridinyl]-1naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-16-4 HCAPLUS

CN Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-18-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-UN'-[4-[6-[(2,6-dimethyl-4-morpholinyl)methyl]-3-pyridinyl]-1-naphthalenyl]-N(9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-20-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methoxy-3-pyridinyl)-1H-pyrazol-5-yl]-UN'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-22-2 HCAPLUS

Urea, N-[1-(6-amino-3-pyridinyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-24-4 HCAPLUS

CN Morpholine, 4-[[5-[4-[[[[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-D pyrazol-5-yl]amino]carbonyl]amino]-1-naphthalenyl]-2-pyridinyl]carbonyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-26-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-(2-oxa-5-azabicyclo[2.2.1]hept-5-ylmethyl)-3-pyridinyl]-1naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-28-8 HCAPLUS

Urea, N-[4-[4-[[(2-cyanoethyl)(3-pyridinylmethyl)amino]methyl]phenyl]-1naphthalenyl]-N'-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1Hpyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-30-2 HCAPLUS

Urea, N-[4-[4-[[(2-cyanoethyl)[(tetrahydro-2-furanyl)methyl]amino]methyl]p[]
henyl]-1-naphthalenyl]-N'-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-[
1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-32-4 HCAPLUS

=

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-UN'-[4-[4-methoxy-6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

RN 294849-34-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[1-(4-morpholinyl)propyl]-3-pyridinyl]-1-naphthalenyl]- (9CI)
(CA INDEX NAME)

PAGE 2-A

RN 294849-36-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1'-methyl[1,4'-bi-1H-pyrazol]-5-yl]-N'-[4-Li-6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-38-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-1-oxido-2H-thiopyran-4-yl)amino]-3-pyridinyl]-1naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-40-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-2H-pyran-4-yl)amino]-3-pyridinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-42-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[5-[(tetrahydro-2H-thiopyran-4-yl)amino]pyrazinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-44-8 HCAPLUS

CN Acetamide, N-[5-[4-[[[[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-Description pyrazol-5-yl]amino]carbonyl]amino]-1-naphthalenyl]-2-pyridinyl]- (9CI)

(CA INDEX NAME)

RN 294849-46-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1'-[3-(methylthio)propyl][1,4'-bi-1H-L]

pyrazol]-5-yl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]-

(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-48-2 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(1-oxido-4-thiomorpholinyl)methyl]-3-pyridinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

RN 294849-50-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-2H-pyran-4-yl)amino]-3-pyridinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-52-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-[2-(methylthio)-5-pyrimidinyl]-1H-pyrazol-U5-yl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI)
(CA INDEX NAME)

PAGE 2-A

RN 294849-54-0 HCAPLUS
CN Urea, N-[1-(2-amino-5-pyrimidinyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]CN Urea, N-[1-(2-amino-5-pyrimidinyl)-1H-pyrazol-5-yl]CN Urea, N-[1-(2-amino-5-pyrimidinyl)-1H-pyrazol-5-yl]CN Urea, N-[1-(2-amino-5-pyrimidinyl)-1H-pyrazol-5-yl]CN Urea, N-[1-(2-amino-5-pyrimidinyl)-1H-pyrazol-5-yl]CN Urea, N-[1-(2-amino-5-pyrimidinyl)-1H-pyrazol-5-yl]CN Urea, N-[1-(2-amino-5-pyrimidinyl)-1H-pyrazol-5-yl]CN Urea, N-[1-(2-amino-5-pyrimidinyl)-1H-pyrazol-

N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-56-2 HCAPLUS

CN

Urea, N-[3-(1,1-dimethylethyl)-1'-methyl[1,4'-bi-1H-pyrazol]-5-yl]-N'-[4-[4-[4-(4-morpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-58-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[6-[(tetrahydro-1-oxido-2H-thiopyran-4-yl)amino]-3-pyridinyl]-1naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-60-8 HCAPLUS
CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[6-(4-thiomorpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-62-0 HCAPLUS

ON Morpholine, 4-[[5-[4-[[[[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-L] pyrazol-5-yl]amino]carbonyl]amino]-1-naphthalenyl]-2-pyrimidinyl]carbonyl]-L (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-64-2 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[3-(4-morpholinylmethyl)-5-pyrimidinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-66-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[6-[(1-oxido-4-thiomorpholinyl)methyl]-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-68-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinylmethyl)-5-pyrimidinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294851-79-9 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[3-(4-morpholinyl)-1-cyclohexen-1-yl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294851-81-3 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[4-(4-morpholinyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294851-83-5 HCAPLUS

Urea, N-[4-[4-[(dimethylamino)methyl]phenyl]-1-naphthalenyl]-N'-[3-(1,1dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 294851-85-7 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-L]
[3-(4-morpholinyl)-1-cyclohepten-1-yl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-L] [3-(4-morpholinyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

IT 261711-84-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of arom. heterocyclic urea antiinflammatory agents by conversion of arylamines to isocyanates followed by addn. of heterocyclic amines)

RN 261711-84-6 HCAPLUS

CN Carbamic acid, [5-(1,1-dimethylethyl)-2-methylphenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L26 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

ER: 2000:493269 HCAPLUS

Patent

DOCUMENT NUMBER: 133:105343

TITLE: Preparation of β -phenylalanine derivatives as

integrin antagonists

INVENTOR(S): Schoop, Andreas; Muller, Gerhard; Bruggemeier, Ulf;

Schmidt, Delf; Stelte-Ludwig, Beatrix; Keldenich,

Jorg; Albers, Markus

PATENT ASSIGNEE(S): Bayer A.-G., Germany SOURCE: PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Pa

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE					
WO 2000041469	A2	20000720	WO 2000-EP120	20000111					
WO 2000041469	A3	20001116		THE STATE OF STATE					
W: AE, AL,	AM, AT	, AU, AZ, BA,	BB, BG, BR, BY, CA	CH, CN, CR, CO,					

```
CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                              19990115
                                            US 1999-232738
                       B1
                            20010918
    US 6291503
                                            CA 2000-2360356
                                                              20000111
                       AA
                            20000720
    CA 2360356
                                                              20000111
                                            EP 2000-903571
                            20011024
                       A2
    EP 1147079
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                                            JP 2000-593094
                                                              20000111
                       T2
                            20021015
     JP 2002534439
                                                              20010530
                                            US 2001-867835
                            20011018
    US 2001031788
                       A1
                            20030708
                       B2
     US 6589972
                                                              19990115
                                         US 1999-232738
PRIORITY APPLN. INFO.:
                                                              20000111
                                                           W
                                         WO 2000-EP120
                         MARPAT 133:105343
OTHER SOURCE(S):
GΙ
```

 β -Phenylalanine derivs. I [R1 = H, (un) substituted alkyl, cycloalkyl, ABaryl, heterocyclyl; R2, R3 = any group given for R1 or (un)substituted alkenyl or alkynyl, OH, alkoxy or R2 and R3 are bonded to each other; R4 = carboxy ester, SO2H, CHO, CONH2, C(S)NH2 or their derivs.; R5 = H, (un) substituted alkyl, cycloalkyl, aryl; R6 = any group given for R1 or is bonded to one of R7, R8 or R9; R7 is absent, H, (un)substituted alkyl or cycloalkyl, NO2, CN, CHO or CO2H or their derivs., or is bonded to one of R6, R8, or R9; R8, R9 = any group given for R1 or is bonded to one of R6, R7 or R9 or R8; R10, R11 = H, (un)substituted alkyl, cycloalkyl, or alkoxy, halo; L is a sulfonamide, amide, ether, ester, keto, urea, thioether, sulfoxide or sulfone unit optionally extended by one or two methylene groups; X is N, O or S] and their physiol. acceptable salts and stereoisomers were prepd. Thus, 3-[(phenylsulfonyl)amino]-3-[3-[(3guanidinophenyl)sulfonyl]phenyl]propionic acid trifluoroacetic acid salt, prepd. by a multistep procedure from 3-nitrobenzaldehyde, ammonium acetate, malonic acid, benzenesulfonyl chloride, 3-nitrobenzenesulfonyl chloride, and 1,3-bis(tert-butoxycarbonyl)-2-methyl-2-thiopseudourea, showed IC50 = 19 nM antagonist activity against integrin $\alpha v \beta 3$ receptor.

IT 283613-04-7P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of β -phenylalanine derivs. as integrin antagonists)

RN 283613-04-7 HCAPLUS

Benzenepropanoic acid, 3-[[[3-[[(1H-benzimidazol-2-ylamino)carbonyl]amino]phenyl]sulfonyl]amino]-β[[(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

IT 283613-53-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of β -phenylalanine derivs. as integrin antagonists)

Benzenepropanoic acid, 3-[[[3-[(ethoxythioxomethyl)amino]phenyl]sulfonyl]a RNmino]- β -[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME) CN

COPYRIGHT 2004 ACS on STN HCAPLUS L26 ANSWER 10 OF 21

Citing Full References

ACCESSION NUMBER:

2000:401817 HCAPLUS

DOCUMENT NUMBER:

133:30667

TITLE:

Heteroaryl-containing thiourea derivatives useful as

inhibitors of herpes viruses

INVENTOR(S):

Bloom, Jonathan David; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; O'Hara,

Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

PCT Int. Appl., 164 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

SOURCE:

FAMILY ACC. NUM. COUNT:

									_				
PATENT NO.		KIND DA	ATE			PLIC	. -	- -	. _ -				
CZ, MD, SK.	DE, IS, MG, SL,	AM, AT, ADK, DM, DK, DM, DM, ME, MN, MN, TJ, TM,	EE, ES, KG, KP, MW, MX, TR, TT,	KR, NO, TZ,	BB, GB, KZ,	BG, GD, LC,	BR, GE, LK,	BY, GH, LR,	CA, GM, LS, RU,	LT, SD,	CN, HU, LU, SE,	LV, SG,	MA, SI,
BY, RW: GH,	KG,	KZ, MD, KE, LS, FI, FR, CM, GA,	RU, TJ, MW, SD,	SL, IE, ML,	SZ, IT, MR, U	TZ, LU,	UG, MC, SN, 99-4	ZW, NL, TD, 4478	AT, PT, TG 2	BE,	CH, BF,	CY, BJ,	DE,

OTHER SOURCE(S):

MARPAT 133:30667

GΙ

$$R^4$$
 R^5
 R^3
 $HN-A-NH$
 G
 R^2
 R^3
 R^3

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 ABalkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 \neq H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; A = heteroaryl; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = aryl or heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and

-7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 25 compds. in 2-4 bioassays. For instance, the pyridinylthiazolecarboxamide deriv. II had an IC50 of 0.001 $\mu g/mL$ against HCMV wild-type in human foreskin fibroblast cell culture.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of heteroaryl-contg. thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RN

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CNester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$Me - S = 0$$

$$C - NH - C - 0Bu - t$$

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of heteroaryl-contg. thiourea derivs. as inhibitors of herpes viruses)

71026-66-9 HCAPLUS

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CNNAME)

$$\begin{array}{c} 0 \\ \parallel \\ \text{NH} - C - 0 \text{Bu-t} \end{array}$$

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compd.; prepn. of heteroaryl-contg. thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME) CN

HCAPLUS 273390-92-4 RN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-CNimidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & & & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

COPYRIGHT 2004 ACS on STN ANSWER 11 OF 21 HCAPLUS L26

2

Citing Full References Text

ACCESSION NUMBER:

2000:401816 HCAPLUS

DOCUMENT NUMBER:

133:30666

TITLE:

Aryl- and heteroaryl-substituted thiourea derivatives

useful as inhibitors of herpes viruses

INVENTOR(S):

Bloom, Jonathan David; Digrandi, Martin Joseph;

Dushin, Russell George; Lang, Stanley Albert; O'Hara,

Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

PCT Int. Appl., 159 pp.

SOURCE:

CODEN: PIXXD2 Patent

DOCUMENT TYPE:

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT NO.				KIND DATE					APPLICATION NO. DATE								
WO 200	00342	68	A:	1 :	20000	0615		W	0 19	99-U	S288	38	1999:	1206			
W ·	AE,	AT.	AM.	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,	
,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	CZ	DE	DK.	DM.	EE.	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	
	TM	TS,	JP.	KE.	KG.	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	
	MD,	MG	MK.	MN.	MW.	MX.	NO.	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	
	SK.	SL.	TJ,	TM,	TR,	TT,	TZ,	UA,	ŪĠ,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	
	BY.	KG.	KZ.	MD,	RU,	TJ,	TM										
RV	7: GH,	GM.	KE.	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	
201	DK.	ES.	FI.	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 19991206 BR 1999-15993 20010904 Α BR 9915993 EP 1999-965131 19991206 20011004 **A**1 EP 1137647 CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, R: AT, BE, IE, SI, LT, LV, FI, RO 19991206 JP 2000-586715 JP 2002531557 20020924 T220010525 ZA 2001-4318 20020826 Α ZA 2001004318 20010608 NO 2001-2837 20010719 Α NO 2001002837 A 19981209 US 1998-207961 PRIORITY APPLN. INFO.: 19991206 WO 1999-US28838 MARPAT 133:30666

OTHER SOURCE(S):

GΙ

$$\begin{array}{c|c} & & & \\ & & &$$

Title compds. I and related compds. and their pharmaceutical salts are ABdisclosed [wherein A = heteroaryl; R1-R4 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, cyano; R1R2 or R3R4 = C5-7 aryl fusion; G = aryl or heteroaryl; and X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph or PhCH2; n =The compds. are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), and varicella-zoster virus (VZV), as well as (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 35 compds. in 2-4 bioassays. For instance, the pyridine deriv. II had an IC50 of 0.018 $\mu g/mL$ against HCMV wild-type in human foreskin fibroblast cell culture.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of heteroaryl thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RN

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CNester (9CI) (CA INDEX NAME)

RN 273384-74-0 HCAPLUS

CN Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} 0 \\ \text{Me} - S \\ \hline \\ C - NH \end{array}$$

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of heteroaryl thiourea derivs. as inhibitors of herpes viruses)

RN 71026-66-9 HCAPLUS

CN Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of heteroaryl thiourea derivs. as inhibitors of herpes viruses)

RN 273390-64-0 HCAPLUS

CN Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

RN 273390-92-4 HCAPLUS

CN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CN yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

COPYRIGHT 2004 ACS on STN HCAPLUS L26 ANSWER 12 OF 21

1

Citing Full References Text

ACCESSION NUMBER:

DOCUMENT NUMBER:

INVENTOR(S):

TITLE:

2000:401809 HCAPLUS

133:30657

Heterocyclic carboxamide-containing thiourea

derivatives containing a substituted phenylenediamine

group, useful as inhibitors of herpes viruses

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Jones, Thomas

Richard; Lang, Stanley Albert; Ross, Adma Antonia; Terefenko, Eugene Anthony; O'Hara, Bryan Mark

American Home Products Corporation, USA

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM.

PATENT NO.	KIND DATE	APPLICATION NO. DATE
WO 2000034261	A2 20000615	WO 1999-US28916 19991206
W: AE, AL, CZ, DE, IN, IS,	JP, KE, KG, KP,	BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
BY, KG, RW: GH, GM, DK, ES,	KZ, MD, RU, TJ, KE, LS, MW, SD, FI, FR, GB, GR, CM, GA, GN, GW,	TM SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, ML, MR, NE, SN, TD, TG
US 6166028 US 6197803 US 6201013 EP 1144399	A 20001226 B1 20010306 B1 20010313 A2 20011017	US 1999-444782 19991122 US 1999-447006 19991122 US 1999-444075 19991122 EP 1999-967213 19991206
EP 1144399 R: AT, BE,	A3 20020911 , CH, DE, DK, ES,	FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, L	r, LV,	FI, RO		
BR 9916043	A	20011204	BR 1999-16043	19991206
JP 2002533301	T2	20021008	JP 2000-586708	19991206
US 6262082	B1	20010717	US 2000-669483	20000925
US 6271236	B1	20010807	US 2000-669943	20000926
ZA 2001004322	A	20021025	ZA 2001-4322	20010525
NO 2001004322	A	20010719	NO 2001-2835	20010608
US 2003036653	A1	20030220	US 2002-99695	20020315
US 6555561	B2	20030429		
PRIORITY APPLN. INFO.:	22		US 1998-208164 A	19981209
PRIORITI APPEN. INTO			US 1998-150692P P	19981209
			US 1998-150698P P	19981209
			US 1998-155192P P	19981209
			US 1998-155240P P	19981209
			US 1998-208540 A	19981209
			US 1998-208561 A	19981209
			US 1999-444782 A3	19991122
			WO 1999-US28916 W	19991206
			US 2000-669535 A3	20000926

OTHER SOURCE(S):

MARPAT 133:30657

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 ABalkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 ≠ H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl fusion, provided that at least 1 of R9-R12 \neq H; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std.

methods are listed, with biol. data for 18 compds. in 4 bioassays. For instance, the N-(4-thioureidophenyl)furan-2-carboxamide deriv. II had an IC50 of 0.4 $\mu g/mL$ against HCMV wild-type in human foreskin fibroblast cell culture, and 0.5 $\mu g/mL$ against HSV in an ELISA assay.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of heterocyclic carboxamide-contg. and phenylenediamine-contg. thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RN

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CNester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Me
$$-S$$

$$C-NH$$

$$NH-C-0Bu-t$$

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of heterocyclic carboxamide-contg. and phenylenediamine-contg. thiourea derivs. as inhibitors of herpes

71026-66-9 HCAPLUS RN

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CNNAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compd.; prepn. of heterocyclic carboxamide-contg. and phenylenediamine-contg. thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

Benzamide, N-[4-[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CN yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

RN 273390-92-4 HCAPLUS

CN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ & & & & & \\ N & & & & \\ N & & \\ \end{array}$$

RN 273390-93-5 HCAPLUS

CN 2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

L26 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

2000:401808 HCAPLUS

DOCUMENT NUMBER:

133:30588

TITLE:

Alpha-methylbenzyl-containing thiourea derivatives

containing a phenylenediamine group, useful as

inhibitors of herpes viruses

INVENTOR(S):

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; Norton, Emily Boucher; Ross, Adma Antonia;

O'Hara, Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

SOURCE:

PCT Int. Appl., 168 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

PATENT NO.	KIND DAT	TE AF	APPLICATION NO. DATE							
WO 2000034260 WO 2000034260	A3 200	000908	1999-US28839	19991206						
W: AE, AL, CZ, DE, IN, IS, MD, MG.	AM, AT, AU DK, DM, EE JP, KE, KG MK, MN, MW	U, AZ, BA, BB, E, ES, FI, GB, G, KP, KR, KZ, W, MX, NO, NZ,	GD, GE, GH, GM LC, LK, LR, LS PL, PT, RO, RU	, CH, CN, CR, CU, , HR, HU, ID, IL, , LT, LU, LV, MA, , SD, SE, SG, SI, , ZA, ZW, AM, AZ,						

```
BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                              19991206
                                            BR 1999-16084
                             20010904
                       Α
    BR 9916084
                                                              19991206
                                            EP 1999-963022
                             20011004
                       A2
     EP 1137645
                             20040526
                       Bl
     EP 1137645
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                                                              19991206
                                             JP 2000-586707
                             20020924
                        T2
     JP 2002531555
                                                              20010528
                                             ZA 2001-4376
                             20020828
                        Α
     ZA 2001004376
                                                              20010608
                                             NO 2001-2833
                             20010802
                        A
     NO 2001002833
                                                              19981209
                                         US 1998-208902
PRIORITY APPLN. INFO.:
                                                              19991206
                                          WO 1999-US28839
                          MARPAT 133:30588
```

OTHER SOURCE(S):

GΙ

$$R^{4}$$
 R^{5}
 R^{9}
 R^{10}
 R^{1

$$\operatorname{Br} \longrightarrow \operatorname{HN} \longrightarrow \operatorname{NH} \longrightarrow \operatorname{II}$$

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 ABalkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 \neq H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl fusion; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = aryl or fused bicyclic aryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 320 compds. in 1-4 bioassays. For instance, the [[(phenylethyl)thioureido]phenyl]benzofurancarboxamide deriv. II had an IC50 of 1.3 $\mu\text{g/mL}$ against HCMV wild-type in human foreskin fibroblast cell culture, and 0.10 $\mu\text{g/mL}$ against VZV in an ELISA assay.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent) (intermediate; prepn. of $\alpha\text{-methylbenzyl-contg.}$ thiourea derivs. as inhibitors of herpes viruses) 273384-69-3 HCAPLUS Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$Me - S = 0$$

$$C - NH - C - 0Bu - t$$

IT 71026-66-9

RN

CN

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of $\alpha\text{-methylbenzyl-contg.}$ thiourea derivs. as inhibitors of herpes viruses)

71026-66-9 HCAPLUS RN

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CNNAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of $\alpha\text{-methylbenzyl-contg.}$ thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c} t-Bu\\ N\\ N\\ N\\ N\\ N\\ \end{array}$$

273390-92-4 HCAPLUS RN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-CN

imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

COPYRIGHT 2004 ACS on STN HCAPLUS ANSWER 14 OF 21 L26

Citing Full References Text ACCESSION NUMBER:

2000:401806 HCAPLUS

DOCUMENT NUMBER:

INVENTOR(S):

133:30733

TITLE:

Heterocyclic carboxamide-containing thiourea derivatives containing a phenylenediamine group,

useful as inhibitors of herpes viruses

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Jones, Thomas

Richard; Lang, Stanley Albert; Ross, Adma Antonia; Terefenko, Eugene Anthony; O'Hara, Bryan Mark

American Home Products Corporation, USA

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 188 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT NO.	KIND DATE	APPLICATION NO. DATE
WO 2000034258 W: AE, AL, CZ, DE, IN, IS,	JP, KE, KG, KP,	WO 1999-US28842 19991206 BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, WG, WG, WG, WG, WH, WH, ZA, ZW, AM, AZ,
SK, SL,	TJ, TM, TR, TT,	TZ, UA, UG, UZ, VN, 10, ZA, ZW, 121,
BY, KG, RW: GH, GM,	KZ, MD, RU, TJ, KE, LS, MW, SD, FI, FR, GB, GR, CM, GA, GN, GW,	TM SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, ML, MR, NE, SN, TD, TG
BR 9916046	A 20011002 A2 20011017	DR 1999 10001206
EP 1144397 R: AT, BE,	72 20020911	

TR 200101664	Т2	20020321	TR 2001-20010166	419991206
JP 2002531554	T2	20020924	JP 2000-586705	19991206
ZA 2001004377	A	20021220	ZA 2001-4377	20010528
NO 2001002832	A	20010807	NO 2001-2832	20010608
BG 105581	A	20011231	BG 2001-105581	20010608
PRIORITY APPLN. INFO.:			US 1998-208559 A	19981209
I KI OKI I I I I I I I I I I I I I I I I			WO 1999-US28842 W	19991206

OTHER SOURCE(S):

MARPAT 133:30733

GI

$$R^4$$
 R^5
 R^5
 R^7
 R^7

$$F3C$$

$$HN$$

$$S$$

$$0$$

$$N=N$$

$$II$$

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 AB alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 \neq H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; W = 0, NR6, or bond; Y =CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 350 compds. in 1-4 bioassays. For instance, the thioureidophenylthiadiazolecarboxamide deriv. II had an IC50 of 0.0011 $\mu g/mL$ against HCMV wild-type in human foreskin fibroblast cell culture.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of heterocyclic carboxamide-contg. thiourea derivs. as inhibitors of herpes viruses)

RN 273384-69-3 HCAPLUS

CN Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} 0 \\ \text{Me} - S \\ \hline \\ C - \text{NH} \end{array}$$

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of heterocyclic carboxamide-contg. thiourea derivs. as inhibitors of herpes viruses)

71026-66-9 HCAPLUS RN

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CNNAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of heterocyclic carboxamide-contg. thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CN yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c} t-Bu\\ \\ N\\ \\ N\end{array}$$

273390-92-4 HCAPLUS RN

CN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1Himidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing Full References Text

ACCESSION NUMBER:

2000:401786 HCAPLUS

DOCUMENT NUMBER:

133:30587

TITLE:

Benzamide-containing aryl thiourea derivatives useful

as inhibitors of herpes viruses

INVENTOR(S):

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley

Albert; Norton, Emily Boucher; Ross, Adma Antonia;

O'Hara, Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

SOURCE:

PCT Int. Appl., 169 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 3

PAT	ENT 1	10.		KIND DATE APPLICATION NO. DATE													
WO	2000	 03423	38	A.	 1	20000	615		WC) 199	99-US	32883	37	1999	1206	an.	OLI.
	W:	$\nabla \mathbf{E}$	7\ T .	ΔM	ΔT	AU.	AZ.	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CIV,	CR,	CU,
		C7	DE	DK.	DM.	EE.	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HK,	пU,	ΙD,	11,
		TNT	TS	JP.	KE.	KG.	KP,	KR,	KZ,	LC,	LK,	LR,	ьs,	mT.	ъU,	ъ∨,	MIA,
		MD	MC	MK	MN	MW.	MX.	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	51,
		SK.	SL.	TJ.	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,
		DV	KG	K7.	MD.	RU.	TJ.	TM									
	DW.	CU	CM	KE	LS	MW.	SD.	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,
	KW.	DK	ES	FT	FR.	GB,	GR.	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
		CC,	CT	CM	GA.	GN,	GW.	ML.	MR,	NE,	SN,	TD,	TG				
110	C1 CC			7	OH,	2000	1226	,	U.	s 19	99-4	4478	2	1999	1122		
<u>US</u>	6166 6197	020		<u> </u>	1	2001	0306		U	S 19	99-4	4700	6	1999	1122		
						2001				S 19	99-4	4407	 5	1999	1122		
	6201				_	2001				······	99-4			1999	1122		
	6207					2001					99-4			1999	1122		
	6255			В							99-4			1999			
	6262			В		2001								1999			
	<u>6335</u>			В		2002					99-4		_	1999			
BR	9916	086		A		2001							•	1999			
\mathbf{EP}_{-}	1137	632		A	.1	2001											рт
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	ГŢ,	ъU,	ИL,	DE,	IVIC,	Р1,

IE, SI, LI	r, LV,	FI, RO			
TR 200101597	T2	20011022	TR 2001-200101		
JP 2002531545	T2	20020924	JP 2000-586686	•	19991206
NZ 512108	A	20030926	NZ 1999-512108	-	19991206
US 6262082	B1	20010717	US 2000-669483		20000925
US 6271236	В1	20010807	US 2000-669943	_	20000926
US 6403617	B1	20020611	US 2000-669535	_	20000926
US 6407123	B1	20020618	US 2000-670180)	20000926
US 6426355	B1	20020730	US 2000-671486	_	20000927
US 6407249	B1	20020618	US 2000-684011		20001229
US 6410571	B1	20020625	US 2000-684773	-	20001229
US 2002026055	A1	20020228	US 2001-804510)	20010312
US 6380243	B2	20020430			
US 2001039348	A1	20011108	US 2001-845428	3	20010430
US 6462055	B2	20021008			
ZA 2001004144	A	20020821	ZA 2001-4144		20010521
NO 2001002838	A	20010808	NO 2001-2838		20010608
BG 105583	A	20011231	BG 2001-105583	3	20010608
US 2003036653	A1	20030220	US 2002-99695		20020315
US 6555561	B2	20030429			
PRIORITY APPLN. INFO.:			US 1998-208561	Α	19981209
			US 1998-228805P	P	19981209
			US 1998-228808P	P	19981209
			US 1998-228809P	P	19981209
			US 1998-150692P	P	19981209
			US 1998-150698P	P	19981209
			US 1998-155192P	P	19981209
			US 1998-155240P	P	19981209
			US 1998-208164	A	19981209
			US 1998-208540	A	19981209
			US 1999-444734	A3	19991122
			US 1999-444782	A3	19991122
			US 1999-444896	A3	19991122
			US 1999-447006	A3	19991122
			WO 1999-US28837	W	19991206
			US 2000-669535	A3	20000926

OTHER SOURCE(S):

MARPAT 133:30587

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8,

NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 ≠ H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl fusion, provided that at least 1 of R9-R12 \neq H; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G =aryl or fused bicyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 75 compds. in 2-4 bioassays. For instance, the thioureidophenylbenzamide deriv. II had an IC50 of 1.5 $\mu g/mL$ against HCMV wild-type in human foreskin fibroblast cell culture, and 0.04 $\mu g/mL$ against HSV in an ELISA assay.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of benzamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

RN 273384-69-3 HCAPLUS

CN Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 273384-74-0 HCAPLUS

CN Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$Me - S = 0$$

$$C - NH - C - 0Bu - t$$

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prepn. of benzamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

RN 71026-66-9 HCAPLUS

CN Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of benzamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

RN 273390-64-0 HCAPLUS

CN Benzamide, N-[4-[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c} t^{-Bu} \\ \downarrow \\ N \\ N \\ \end{array} \qquad \begin{array}{c} N \\ N \\ N \\ \end{array} \qquad \begin{array}{c} N \\ N \\ N \\ \end{array} \qquad \begin{array}{c} N \\ N \\ \end{array} \qquad$$

RN 273390-92-4 HCAPLUS

CN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & & & & \\ & & & \\ N & & & \\ N & & \\ N$$

RN 273390-93-5 HCAPLUS

CN 2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & & & \\ & & & \\$$

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

2000:401785 HCAPLUS

133:30586

4

DOCUMENT NUMBER: TITLE:

Acetamide and substituted acetamide-containing aryl thiourea derivatives useful as inhibitors of herpes

viruses

INVENTOR(S):

Bloom, Jonathan David; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; O'Hara,

Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

SOURCE:

PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

DATE APPLICATION NO. KIND DATE PATENT NO. 19991206 WO 1999-US28844 20000615 **A**2 WO 2000034237 20001123 WO 2000034237 A3W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG EP 1999-965132 19991206 20011004 A2 EP 1137633 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO 19991206 BR 1999-16041 20011204 \mathbf{A} BR 9916041 JP 2000-586685 19991206 T2 20020924 JP 2002531544 20010521 ZA 2001-4142 20021025 Α ZA 2001004142 20010608 NO 2001-2834 20010807 Α NO 2001002834 A 19981209 US 1998-208316 PRIORITY APPLN. INFO.: 19991206 WO 1999-US28844 W MARPAT 133:30586

OTHER SOURCE(S):

GI

$$R^4$$
 R^5
 R^9
 R^{10}
 R^3
 R^4
 R^5
 R^9
 R^{10}
 R^9
 R^9
 R^{10}
 R^9
 R

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 AB alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 ≠ H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl

fusion; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = C1-6 alkyl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 160 compds. in 4 bioassays. For instance, the thioureidophenylacetamide deriv. II had an IC50 of 0.8 $\mu g/mL$ against HCMV wild-type in human foreskin fibroblast cell culture, and 2 $\mu g/mL$ against HSV in an ELISA assay.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of acetamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

RN 273384-69-3 HCAPLUS

CN Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 273384-74-0 HCAPLUS

CN Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prepn. of acetamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

RN 71026-66-9 HCAPLUS

CN Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compd.; prepn. of acetamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

CN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

273390-92-4 HCAPLUS RN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-CNimidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CN yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L26

Citing Full References Text

ACCESSION NUMBER: DOCUMENT NUMBER:

TITLE:

2000:335391 HCAPLUS

132:347569

Preparation gastrin and cholecystokinin receptor

ligands

INVENTOR(S):

Kalindjian, Sarkis Barret; Buck, Ildiko Maria; Linney, Ian Duncan; Wright, Paul Trevor; McDonald, Iain Mair; Steel, Katherine Isobel Mary; Hull, Robert Antony David; Roberts, Sonia Patricia; Gaffen, John David; Vinter, Jeremy Gilbert; Walker, Martin Keith; Black, James Whyte; Watt, Gillian Fairfull; Harper, Elaine Anne; Shankley, Nigel Paul; Tozer, Matthew John; Dunstone, David John; Pether, Michael John; Lilley, Elliot James; Sykes, David Andrew; Low, Caroline Minli Rachel; Griffin, Eric Peter; Wright, Laurence

PATENT ASSIGNEE(S):

SOURCE:

James Black Foundation Limited, UK

PCT Int. Appl., 210 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

GΙ

```
APPLICATION NO.
                                                            DATE
                     KIND DATE
    PATENT NO.
                                           WO 1999-GB3733
                      A1
                            20000518
    WO 2000027823
           AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
            CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
            IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
            MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
            SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
            DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
            CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                           CA 1999-2346108
                                                            19991109
                            20000518
                      AA
    CA 2346108
                                                            19991109
                                           BR 1999-15194
                            20010807
                      Α
    BR 9915194
                                           EP 1999-954196
                                                            19991109
                            20020213
                      A1
    EP 1178969
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO
                                           JP 2000-581003
                                                            19991109
                       T2
                            20020910
    JP 2002529455
                                                            20010509
                                           NO 2001-2288
    NO 2001002288
                            20010702
                      Α
                                           US 2001-831385
                                                            20010802
                            20021112
                       В1
    US 6479531
                                                         A 19981109
                                        GB 1998-24536
PRIORITY APPLN. INFO.:
                                                         A 19990716
                                        GB 1999-16786
                                                            19991109
                                        WO 1999-GB3733
                       MARPAT 132:347569
OTHER SOURCE(S):
```

Title compds. (I) [wherein X and Y = independently N, N(R5), CH, S, or O; ABn = 1-4; Z = (NR7)aCO(NR8)b, CONR7CH2CONR8, CO2, CH2CH2, CH=CH, CH2N(R8), or a bond; a and b = independently 0 or 1; Q = R9V (un) substituted phenyl(alkyl); V = CONHSO2Ph, SO2NHCOPh, CH2OH, etc.; R1 = H or (halo) hydrocarbyl where \leq 3 C atoms may be replaced by N, O, and/or S atoms; R2 = H, Me, Et, Pr, or OH; R3 = H, Me, Et, or Pr; or 2 adjacent R3 groups form a carbocyclic ring when n > 1; or R2 and R3 on the same C atom together = :0 ; R4 = $(halo) hydrocarbyl where \le 2 C atoms may$ be replaced by N, O, and/or S atoms; R5 = H, Me, Et, Pr, benzyl, OH, or carboxymethyl (esters); R7 and R8 = independently H, Me, Et, Pr, or benzyl; R9 = CH2, CH2CH2, or (un) substituted phenylmethylene; or R8 and R9, together with the adjacent N, form a substituted piperidine or pyrrolidine] and their pharmaceutically acceptable salts were prepd. Examples include syntheses and biol. data for 314 compds. Thus, 2-adamantan-1-ylmethyl-5-phenyl-1H-pyrrole-3-carboxylic acid (3-step prepn. given) was coupled with 5-aminoisophthalic acid dibenzyl ester (45%), followed by deprotection (98%) to give II. II had pKi of 6.72 for binding at the CCKB mouse cortical membranes and pKb of 6.33 for gastrin antagonist activity.

IT 269071-04-7P 269071-45-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. gastrin and cholecystokinin receptor ligands)

RN 269071-04-7 HCAPLUS

CN Benzoic acid, 3-[[[[2-(2-methylphenyl)-5-(2-tricyclo[3.3.1.13,7]dec-1-ylethyl)-1H-imidazol-4-yl]amino]carbonyl]amino]-, phenylmethyl ester (9CI)

(CA INDEX NAME)

RN 269071-45-6 HCAPLUS

CN Benzoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-[[[2-(2-methylphenyl)-5-(2-tricyclo[3.3.1.13,7]dec-1-ylethyl)-1H-imidazol-4-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

IT 269072-17-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. gastrin and cholecystokinin receptor ligands)

RN 269072-17-5 HCAPLUS
CN Benzoic acid, 5-amino-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CN

IT 269068-26-0P 269073-03-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. gastrin and cholecystokinin receptor ligands)

269068-26-0 HCAPLUS RN

Benzoic acid, 3-[[[[2-(2-methylphenyl)-5-(2-tricyclo[3.3.1.13,7]dec-1ylethyl)-1H-imidazol-4-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

269073-03-2 HCAPLUS RN

D-Glucitol, 1-deoxy-1-(methylamino)-, 3-[[[[2-(2-methylphenyl)-5-(2-CNtricyclo[3.3.1.13,7]dec-1-ylethyl)-1H-imidazol-4yl]amino]carbonyl]amino]benzoate (salt) (9CI) (CA INDEX NAME)

CM1

269068-26-0 CRN C30 H34 N4 O3 CMF

CRN 6284-40-8 CMF C7 H17 N O5

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L26

4

Citing Full References Text

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

1999:425745 HCAPLUS

131:87909

Inhibition of p38 kinase activity using substituted

heterocyclic ureas

INVENTOR (S):

Dumas, Jacques; Khire, Uday; Lowinger, Timothy Bruno; Paulsen, Holger; Riedl, Bernd; Scott, William J.;

Smith, Roger A.; Wood, Jill E.; Hatoum-Mokdad, Holia;

Johnson, Jeffrey; Lee, Wendy; Redman, Aniko

PATENT ASSIGNEE(S):

SOURCE:

Bayer Corporation, USA

PCT Int. Appl., 126 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PA	TENT			KIND DATE APPLICATION NO. DATE														
WO	9932	111		A	1	 1999:	0701		W	O 19	98-U	5260	80	1998	1222			
	W :	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,	
		DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	
		KE.	KG.	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	
		MW.	MX.	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	
		TR.	TT.	UA.	UG.	UZ,	VN,	YU,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM
	RW.	GH.	GM.	KE.	LS.	MW.	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,	ES,	
	1000	FT.	FR.	GB.	GR.	IE.	IT.	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	
						ML,						-						
$C\Delta$	2315	720	011,	Δ1,	Δ.,	1999	0701		C	A 19	98-2	3157	20	1998	1222			
711	9919	971		A	1	1999	0712		$\overline{\mathbf{A}}$	U 19	99-1	9971	,,.	1998	1222			
	7396								-									
	1041								E	P 19	98-9	6470	9	1998	1222			
<u> </u>		70Z	מם	CH	DE.	ראר האר	ES	ਸ਼ਸ	GB.	GR.	IT.	LI.	LU,	NL,	SE,	MC,	PT,	
	R:					FI,		110,	00,		,	,	,	,	- ,	•	•	
TP	2001	TE,	эт,	тт,	лv,	2001	1219		Τ.	P 20	00-5	2510	2	1998	1222			
PRIORIT	2001	.5202	<u> </u>	1	2	2001	1210		110 1	997-	9957	50	Σ					
PRIORIT	Y APE	,ГИ .	INFO	. :					MO 1	998-	11526	080	W	1998	1222			
							1			<i>JJ</i> 0-	0520	000	**	1990	1222			
OTHER S	OURCE	E(S):			MAR	TPAT	T3T:	8/90	9									
GI																		

AB A method for treatment of p38-mediated disease other than cancer comprises administration of ANHCONHB [I; A = substituted isoxazolyl, pyrazolyl, thienyl, furyl; B = (substituted) mono-, di-, or tricyclic aryl, heteroaryl contg. ≥1 5-6 membered arom. structure contg. 0-4 N, O, or S atoms]. Reaction of 4-(4-pyridinylthio)aniline with 3-tert-butyl-5-isoxazolyl isocyanate in toluene gave title compd. II. In an in vitro p38 kinase assay, I displayed IC50 values of 1-10 µM.

IT 135680-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of substituted heterocyclic ureas for treatment of p38 kinase-mediated diseases other than cancer)

RN 135680-03-4 HCAPLUS
CN Carbamic acid, [4-[(4-aminophenyl)methyl]phenyl]-, 1,1-dimethylethyl ester
(9CI) (CA INDEX NAME)

IT 229002-05-5P 229003-23-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of substituted heterocyclic ureas for treatment of p38 kinase-mediated diseases other than cancer)

RN 229002-05-5 HCAPLUS

Urea, N-[4-[(4-aminophenyl)methyl]phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu RN 229003-23-0 HCAPLUS

CN 1H-Pyrazole-1-acetic acid, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 229001-93-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229001-95-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-pyridinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229001-97-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

RN 229001-98-3 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[3-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

229002-00-0 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-CN(phenylthio)phenyl] - (9CI) (CA INDEX NAME)

t-Bu

229002-01-1 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-CNhydroxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

229002-02-2 HCAPLUS RN

Urea, N-[4-[(4-butoxyphenyl)thio]phenyl]-N'-[3-(1,1-dimethylethyl)-1-CNmethyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu

229002-03-3 HCAPLUS

RNButanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenyl]methyl]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

t-Bu

229002-04-4 HCAPLUS

RNCarbamic acid, [4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenyl]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME) (9CI)

t-Bu

229002-06-6 HCAPLUS RN

Acetamide, N-[4-[[4-[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

229002-07-7 HCAPLUS RN

Butanoic acid, 4-[[4-[[4-[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenyl]methyl]phenyl]amino]-4-oxo- (9CI) INDEX NAME)

t-Bu

229002-08-8 HCAPLUS

RNPropanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

229002-09-9 HCAPLUS

RN Urea, N-[4-(4-aminophenoxy)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-CNpyrazol-5-yl] - (9CI) (CA INDEX NAME)

t-Bu

229002-10-2 HCAPLUS

RNCN

pyridinyloxy)phenyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & \\ & \\ N \\ & \\ t-Bu \end{array}$$

RN 229002-11-3 HCAPLUS

CN Carbamic acid, [4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NH} - \text{C} - \text{NH} \\ \text{NH} - \text{C} - \text{OEt} \\ \end{array}$$

RN 229002-12-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-pyridinylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-13-5 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-pyridinylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-14-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 229002-15-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229002-16-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-methylphenoxy)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} Me \\ NH-C-NH \\ \end{array}$$

RN 229002-17-9 HCAPLUS

Urea, N-[3-(2-benzothiazolyloxy)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-18-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-phenyl-2-thiazolyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-19-1 HCAPLUS

CN Urea, N-[4-(2-benzothiazolylthio)-3-(trifluoromethyl)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-20-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-(1,1-dimethylethyl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-21-5 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-[4-[(trifluoromethyl)thio]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-22-6 HCAPLUS

Urea, N-[1,1'-biphenyl]-3-yl-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu 22

229002-24-8 HCAPLUS

CN Butanamide, N-[4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 229002-25-9 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-propoxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229002-26-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2,2,2-trifluoroethyl)-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

t-Bu´

RN 229002-27-1 HCAPLUS

CN Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

t-Bu

RN <u>229002-28-2</u> HCAPLUS

CN 1H-Pyrazole-1-carboxylic acid, 3-(1,1-dimethylethyl)-5-[[[[4-[3-[(methylamino)carbonyl]phenoxy]phenyl]amino]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-Bu

RN 229002-87-3 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[[(9H-fluoren-2-ylamino)carbonyl]amino]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 229002-97-5 HCAPLUS

Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-(2-hydroxyethyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-98-6 HCAPLUS

CN 1H-Pyrazole-1-acetic acid, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

RN 229002-99-7 HCAPLUS

CN 1H-Pyrazole-1-acetamide, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)

RN 229155-38-8 HCAPLUS

Urea, N-[4-[(4,5-dihydro-4-phenyl-5-thioxo-1,3,4-thiadiazol-2-yl)thio]phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229155-39-9 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4,5-diphenyl-2-thiazolyl)thio]phenyl]- (9CI) (CA INDEX NAME)

229155-40-2 HCAPLUS RN

Urea, N-[4-([1,1'-biphenyl]-4-yloxy)-3-(trifluoromethyl)phenyl]-N'-[3-(1,1-CNdimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu

229155-41-3 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-CN(phenylmethoxy)phenoxy]phenyl] - (9CI) (CA INDEX NAME)

t-Bu´

229155-42-4 HCAPLUS

RNUrea, N,N''- (methylenedi-4,1-phenylene) bis [N'-[3-(1,1-dimethylethyl)-1-CNmethyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

229155-43-5 HCAPLUS RN

Urea, N,N''-(oxydi-4,1-phenylene)bis[N'-[3-(1,1-dimethylethyl)-1-methyl-1H-CNpyrazol-5-yl] - (9CI) (CA INDEX NAME)

229155-44-6 HCAPLUS RN

Propanamide, N-[4-[4-[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-methyl-5-methyl-5-methyl-5-methyl-5-methyl-5-methyl-5-methyl-5-methyl-5-methyl-5-methyl-5-methylCNyl]amino]carbonyl]amino]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

229155-45-7 HCAPLUS RN

Acetamide, N-[4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu 229155-46-8 HCAPLUS RN

Carbamic acid, [4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenoxy]phenyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NH} - \text{C} - \text{NH} \\ \text{NH} - \text{C} - \text{OPr} - \text{M} \end{array}$$

229155-47-9 HCAPLUS RN

Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-CN5-y1]- (9CI) (CA INDEX NAME)

RN

229155-48-0 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-CN(trifluoromethyl)phenyl] - (9CI) (CA INDEX NAME)

229155-49-1 HCAPLUS RN

Urea, N-(3,5-dibromophenyl)-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-CN5-y1]- (9CI) (CA INDEX NAME)

t-Bu

229155-50-4 HCAPLUS

RNBenzoic acid, 4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CN yl]amino]carbonyl]amino]-, butyl ester (9CI) (CA INDEX NAME)

t-Bu

229155-51-5 HCAPLUS

RNUrea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-CN pyridinylthio)-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

t-Bu

229155-52-6 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-CNpyridazinyl)ethyl]phenyl] - (9CI) (CA INDEX NAME)

t-Bu

229155-53-7 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-CNpyridinylamino)phenyl] - (9CI) (CA INDEX NAME)

t-Bu RN

229155-54-8 **HCAPLUS** CN Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-(2,2,2-trifluoroethyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229155-55-9 HCAPLUS

CN Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(2,3-dichlorophenyl)- (9CI) (CA INDEX NAME)

RN 229155-56-0 HCAPLUS

CN Urea, N-[1-cyclohexyl-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 229155-69-5 HCAPLUS

CN Benzamide, 4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]-N-ethyl- (9CI) (CA INDEX NAME)

RN 229155-70-8 HCAPLUS

CN Benzamide, 4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]thio]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

RN 229155-71-9 HCAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[[3-[[(1-methyl-3-phenyl-1H-pyrazol-5-yl)amino]carbonyl]amino]phenyl]thio]- (9CI) (CA INDEX NAME)

RN <u>229155-81-1</u> HCAPLUS

CN 2-Pyridinecarboxamide, N-methyl-5-[4-[[[(1-methyl-3-phenyl-1H-pyrazol-5-yl)amino]carbonyl]amino]phenoxy] - (9CI) (CA INDEX NAME)

IT 229003-22-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; prepn. of substituted heterocyclic ureas for treatment of p38 kinase-mediated diseases other than cancer)

RN 229003-22-9 HCAPLUS

CN Carbamic acid, (2,3-dichlorophenyl)-, 2-[5-[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)-1H-pyrazol-1-yl]ethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

1

L26 ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing Full References Text

1999:425740 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

131:73648 Inhibition of raf kinase using substituted

heterocyclic ureas

INVENTOR(S):

Dumas, Jacques; Khire, Uday; Lowinger, Timothy Bruno; Paulsen, Holger; Riedl, Bernd; Scott, William J.; Smith, Roger A.; Wood, Jill E.; Hatoum-Mokdad, Holia;

Johnson, Jeffrey; Lee, Wendy; Redman, Aniko

PATENT ASSIGNEE(S):

SOURCE:

LANGUAGE:

GI

Bayer Corporation, USA PCT Int. Appl., 163 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.				KIND DATE					APPLICATION NO.					DATE				
						- 			_	- -		- - -	- -					
WO				A1 19990701				WO 1998-US26078					19981222					
	W:	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,	
		DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	ΙL,	IN,	IS,	JP,	
		KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	
		MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	
														KZ,				TM
	RW:													CY,				
		FI.	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	
							MR,											
CA	2315											3157	17	1998	1222			
AU	AU 9921989		A	A1 19990712				AU 1999-21989 1						1222				
EP	1047	1047418		A1 20001		1102	EP 1998-965981			1	1998	1222						
														ΝL,		MC,	PT,	
							RO											
TR	2000	0261	8	т	2	2001	0420		\mathbf{T}	R 20	00-2	0000	<u> 261</u> 8	1998	1222			
JP	JP 2001526220			Т	2	2001	1218		J	P 20	00-5	2509	7	1998	1222			
BR	9814	374		А		2002	0514		В	R 19	98-1	4374		1998	1222			
NO	2000	0032	32	A		2000	0821		N	0 20	00-3	232		2000	0621			
BG	1045	97		A		2001	0228		В	G 20	00-1	0459	7	2000	0712			
RIORIT														1997				
									WO 1	998-	US26	078	W	1998	1222			
THER S	HER SOURCE(S):				MAR	PAT	131:	7364	8									

A method for treatment of cancerous cell growth mediated by raf kinase ABcomprises administration of urea derivs. ANHCONHB [I; A = substituted isoxazolyl, thienyl, thiadiazolyl, furyl, pyrazolyl, etc.; B = (substituted) mono-, di-, or tricyclic aryl, heteroaryl contg. ≥1 5-6 membered arom. structure contg. 0-4 N, O, or S atoms]. Reaction of 4-phenyloxyphenyl isocyanate with 5-amino-3-tert-butylisoxazole in methylene chloride and heating at reflux temp. for 2 days gave title

compd. II. In an in vitro raf kinase assay, I displayed IC50 values of 1-10 $\mu\text{M}\,.$

IT 135680-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

RN 135680-03-4 HCAPLUS

CN Carbamic acid, [4-[(4-aminophenyl)methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 229002-05-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

RN 229002-05-5 HCAPLUS

CN Urea, N-[4-[(4-aminophenyl)methyl]phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu IT 229001-93-8P 229001-94-9P 229001-95-0P

229001-96-1P 229001-97-2P 229001-98-3P 229001-99-4P 229002-00-0P 229002-01-1P 229002-06-6P 229002-07-7P 229002-08-8P 229002-09-9P 229002-10-2P 229002-11-3P 229002-12-4P 229002-13-5P 229002-11-3P 229002-15-7P 229002-16-8P 229002-17-9P 229002-18-0P 229002-19-1P 229002-20-4P 229002-21-5P 229002-22-6P 229002-23-7P 229002-24-8P 229002-25-9P 229002-26-0P 229002-27-1P 229002-28-2P 229002-85-1P 229002-86-2P 229002-87-3P 229002-97-5P 229002-98-6P 229002-99-7P 229003-04-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

RN 229001-93-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 229001-94-9 HCAPLUS

CN Benzamide, 5-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)

RN 229001-95-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-pyridinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229001-96-1 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-methoxyphenyl)methylamino]phenyl]- (9CI) (CA INDEX NAME)

RN 229001-97-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[3-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

t-Bu 2

229001-99-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[[2-(trifluoromethyl)-4-pyridinyl]thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-00-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)

t-Bu RN

229002-01-1 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-hydroxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

t-Bu RN

229002-02-2 HCAPLUS

CN Urea, N-[4-[(4-butoxyphenyl)thio]phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

CN Butanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \text{t-Bu} \\ \end{array}$$

RN 229002-04-4 HCAPLUS

CN Carbamic acid, [4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 229002-06-6 HCAPLUS

CN Acetamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-07-7 HCAPLUS

Butanoic acid, 4-[[4-[[4-[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

RN 229002-08-8 HCAPLUS

CN Propanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-09-9 HCAPLUS

Urea, N-[4-(4-aminophenoxy)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1Hpyrazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229002-10-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinyloxy)phenyl]- (9CI) (CA INDEX NAME)

t-Bu´

RN 229002-11-3 HCAPLUS

CN Carbamic acid, [4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 229002-12-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-pyridinylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229002-13-5 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-pyridinylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-14-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{OPh} \\ & \text{N} & \text{NH} - \text{C} - \text{NH} \end{array}$$

RN 229002-15-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NH} - \text{C} - \text{NH} \end{array}$$

RN 229002-16-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-methylphenoxy)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & \\ & \\ N \\ & \\ \text{t-Bu} \end{array}$$

RN 229002-17-9 HCAPLUS

CN Urea, N-[3-(2-benzothiazolyloxy)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-18-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-phenyl-

2-thiazolyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-19-1 HCAPLUS

CN Urea, N-[4-(2-benzothiazolylthio)-3-(trifluoromethyl)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-20-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-(1,1-dimethylethyl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & \\ & & \\$$

RN 229002-21-5 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-[4-[(trifluoromethyl)thio]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu RN 229002-22-6 HCAPLUS

CN Urea, N-[1,1'-biphenyl]-3-yl-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-23-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[3-

(phenylmethoxy)phenoxy]phenyl] - (9CI) (CA INDEX NAME)

RN 229002-24-8 HCAPLUS

CN Butanamide, N-[4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 229002-25-9 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-propoxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \\ \text{OPr-n} \end{array}$$

RN 229002-26-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2,2,2-trifluoroethyl)-1H-pyrazol-5-yl]N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 229002-27-1 HCAPLUS

Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 229002-28-2 HCAPLUS

CN 1H-Pyrazole-1-carboxylic acid, 3-(1,1-dimethylethyl)-5-[[[[4-[3-

[(methylamino)carbonyl]phenoxy]phenyl]amino]carbonyl]amino]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 229002-85-1 HCAPLUS

CN Urea, N-(3-cyclopropyl-1-methyl-1H-pyrazol-5-yl)-N'-[4-(6-quinolinyloxy)phenyl]- (9CI) (CA INDEX NAME)

RN 229002-86-2 HCAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[4-[[[(1-methyl-3-phenyl-1H-pyrazol-5-yl)amino]carbonyl]amino]phenoxy] - (9CI) (CA INDEX NAME)

RN 229002-87-3 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[[(9H-fluoren-2-ylamino)carbonyl]amino]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 229002-97-5 HCAPLUS

Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-(2-hydroxyethyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu

RN

229002-98-6 HCAPLUS

1H-Pyrazole-1-acetic acid, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-CN 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

RN

229002-99-7 HCAPLUS

1H-Pyrazole-1-acetamide, 5-[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-CN(1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)

t-Bu

RN229003-04-7 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[3-(4-CNpyridinyloxy)phenyl] - (9CI) (CA INDEX NAME)

IT 229003-22-9 229003-25-2

RL: RCT (Reactant); RACT (Reactant or reagent) (reactant; prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

229003-22-9 HCAPLUS RN

Carbamic acid, (2,3-dichlorophenyl)-, 2-[5-[[(2,3-CNdichlorophenyl) amino] carbonyl] amino] -3 - (1,1-dimethylethyl) -1H-pyrazol-1yl]ethyl ester (9CI) (CA INDEX NAME)

RN 229003-25-2 HCAPLUS

CN Carbamic acid, [4-[4-[[[[5-(1,1-dimethylethyl)-3-isoxazolyl]amino]carbonyl]amino]phenoxy]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1998:402427 HCAPLUS

DOCUMENT NUMBER: 129:81759

TITLE: Preparation and formulation of benzodiazepine

derivatives as gastrin and cholecystokinin antagonists

INVENTOR(S): Shinozaki, Katsuo; Yoneta, Tomoyuki; Murata, Masakazu;

Miura, Naoyoshi; Maeda, Kiyoto

PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan; Shinozaki,

Katsuo;; Yoneta, Tomoyuki;; Murata Masakazu;; Miura,

EP 1997-947872

19971210

Naoyoshi;; Maeda, Kiyoto;

SOURCE: PCT Int. Appl., 432 pp.

A1

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

EP 945445

APPLICATION NO. PATENT NO. KIND DATE DATE WO 1997-JP4534 19971210 WO 9825911 A1 19980618 W: AU, CA, CN, JP, KR, US RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE AU 1998-54100 A1 19980703 19971210 AU 9854100 AU 721081 B2 20000622

19990929

EP	9454	45		B	1	2003	0903										
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	FI														
CN	1246	850		A		2000	0308		Cl	1 199	97-1	8159	9	1997	1210		
CN	1130	351		В		2003	1210										
AT	2488	23		E		2003	0915		ΑT	Γ 199	97-9	4787	2	1997	1210		
PT	9454	45		${f T}$		2004	0130		P	<u>r 199</u>	97-9	4787	2	1997	1210		
ES	2206	754		T	3	2004	0516		ES	3 199	97-9	4787	2	1997	1210		
US	6239	131		B	1	2001	0529		ŪS	3 199	99-3	1924	9	1999	0608		
KR	2000	0575	06	A		2000	0915		KI	R 199	99-7	0519	3	1999	0610		
PRIORIT	Y APP	LN.	INFO	. :				_	JP 19	996-3	3444	98	Α	1996	1210		
									JP 19	997-	1561	32	A	1997	0530		
									WO 19	997-1	JP45	3 <u>4</u>	W	1997	1210		

OTHER SOURCE(S):

MARPAT 129:81759

Ι

GI

The title compds. I [R1 represents hydrogen, lower alkyl, lower alkoxy or halogeno; R2 and R3 may be the same or different and each represents hydrogen, alkenyl, alkyl, Ph, acyl, etc.; and R4 and R5 may be the same or different and each represents hydrogen, alkyl, carboxyl, etc.; Ar = arom. heterocycle, etc.; n = 0 or 2] are prepd. The compds. have an excellent gastrin and/or CCK-B receptor antagonism and are useful as remedies for gastric ulcer and gastrointestinal movement disorder. In an in vitro test for CCK-B receptor antagonism, the title compd. (+)-II showed the Ki value of 1.16 nM. (+)-II at 1 mg/kg intraduodenally gave 81% inhibition of stomach acid secretion induced by pentagastrin 15 μg/kg/h in rats.

Π

IT 209219-48-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzodiazepine derivs. as gastrin and cholecystokinin antagonists)

RN 209219-48-7 HCAPLUS

Urea, N-[5-cyclohexyl-1-(3,3-dimethyl-2-oxobutyl)-2,3,4,5-tetrahydro-2-oxo-1H-1,5-benzodiazepin-3-yl]-N'-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ N & & & \\ N & & \\ N$$

IT 19962-06-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzodiazepine derivs. as gastrin and cholecystokinin antagonists)

RN 19962-06-2 HCAPLUS

CN Carbamic acid, (3-hydroxyphenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 209222-94-6P 209222-95-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of benzodiazepine derivs. as gastrin and cholecystokinin antagonists)

RN 209222-94-6 HCAPLUS

CN Propanoic acid, 2-[3-[[(1,1-dimethylethoxy)carbonyl]amino]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 209222-95-7 HCAPLUS

CN Propanoic acid, 2-[3-[[(1,1-dimethylethoxy)carbonyl]amino]phenoxy]-2-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

1995:709095 HCAPLUS

DOCUMENT NUMBER:

123:218414

TITLE: Imidazoles and antiarteriosclerotics containing the

imidazoles

INVENTOR(S): Kumazawa, Toshiaki; Harakawa, Hiroyuki; Fukui, Hiromi;

Shirokura, Shiro; Ooishi, Eiko; Yamada, Koji

PATENT ASSIGNEE(S):
SOURCE:

Kyowa Hakko Kogyo Kk, Japan Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 07133224 A2 19950523 JP 1993-280961 19931110
PRIORITY APPLN. INFO.: JP 1993-280961 19931110

OTHER SOURCE(S): MARPAT 123:218414

GΙ

AB Antiarteriosclerotics contain imidazoles I [X, Y = CH, N; Z = single bond, CH2; R1, R2, R3 = H, halo, lower alkyl, OH, lower alkoxy, carboxy, lower alkoxycarbonyl, NH2, mono- or di-lower alkyl-substituted amino, carbamoyl, mono- or di-lower alkyl-substituted carbamoyl, CF3; R4, R5, R6 = H, halo, lower alkyl, lower alkoxy; R7 = H, lower alkyl, lower alkyl- (un)substituted cycloalkyl] or their pharmacol. acceptable salts as active ingredients. N-[1-(2-chlorophenyl)-2-benzimidazolyl]-N'-(2,6-diisopropylphenyl)urea (II) (2.3 g) was prepd. by treatment of 1.5 g 2-amino-1-(2-chlorophenyl)benzimidazole and 1.46 mL 2,6-diisopropylphenyl isocyanate. II (at 10-7M) inhibited acyl CoA:cholesterol acyltransferase by 85%. II showed min. LD of >100 mg/kg i.p. in mice. A formulation example of tablets is given.

IT 168120-11-4P 168120-12-5P 168120-13-6P

168120-16-9P 168120-18-1P 168120-21-6P

168120-32-9P

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antiarteriosclerotics contg. imidazoles)

RN <u>168120-11-4</u> HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-(1-phenyl-1H-benzimidazol-2-yl)(9CI) (CA INDEX NAME)

RN <u>168120-12-5</u> HCAPLUS

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-chlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-13-6 HCAPLUS

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(3-chlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & i - Pr \\
 & 0 \\
 & C - NH \\
 & i - Pr \\
 & C - NH \\
 &$$

RN 168120-16-9 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-methylphenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-18-1 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-[2-(dimethylamino)phenyl]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-21-6 HCAPLUS

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2,6-dichlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-32-9 HCAPLUS

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[3-(2-chlorophenyl)-3H-imidazo[4,5-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)

IT 168120-19-2P 168120-27-2P 168120-30-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(antiarteriosclerotics contg. imidazoles)

RN 168120-19-2 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-methoxyphenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-27-2 HCAPLUS

CN Benzoic acid, 3-[2-[[[[2,6-bis(1-methylethyl)phenyl]amino]carbonyl]amino]1H-benzimidazol-1-yl]-4-chloro-, methyl ester (9CI) (CA INDEX NAME)

RN 168120-30-7 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-chlorophenyl)-6-methoxy-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & i\text{-Pr} \\ & 0 \\ & NH-C-NH \\ & i\text{-Pr} \end{array}$$

IT 168120-14-7P 168120-15-8P 168120-17-0P

<u>168120-20-5</u>P <u>168120-22-7</u>P <u>168120-23-8</u>P

168120-24-9P 168120-25-0P 168120-26-1P

168120-28-3P 168120-29-4P 168120-31-8P

168120-33-0P 168120-34-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antiarteriosclerotics contg. imidazoles)

RN 168120-14-7 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(4-chlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-15-8 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-bromophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

HCAPLUS

168120-17-0

RN

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-[2-(trifluoromethyl)phenyl]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-20-5 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-hydroxyphenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-22-7 HCAPLUS

CN Urea, N-[1-(2-chlorophenyl)-1H-benzimidazol-2-yl]-N'-(2,4-difluorophenyl)(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
N & NH - C - NH \\
\hline
\end{array}$$

RN 168120-23-8 HCAPLUS

Urea, N-[1-(2-chlorophenyl)-1H-benzimidazol-2-yl]-N'-(2,6-dimethylphenyl)(9CI) (CA INDEX NAME)

RN 168120-24-9 HCAPLUS

CN Urea, N-[1-(2,6-dichlorophenyl)-1H-benzimidazol-2-yl]-N'-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

RN 168120-25-0 HCAPLUS

CN Urea, N-(2,6-dichlorophenyl)-N'-[1-(2,6-dichlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-26-1 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-[2-chloro-4-(dimethylamino)phenyl]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-28-3 HCAPLUS

CN Benzoic acid, 3-[2-[[[[2,6-bis(1-methylethyl)phenyl]amino]carbonyl]amino]1H-benzimidazol-1-yl]-4-chloro- (9CI) (CA INDEX NAME)

RN 168120-29-4 HCAPLUS

CN 1H-Benzimidazole-6-carboxylic acid, 2-[[[[2,6-bis(1-methylethyl)phenyl]amino]carbonyl]amino]-1-(2-chlorophenyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} i-Pr \\ 0 \\ NH-C-NH \\ i-Pr \\ \end{array}$$

RN 168120-31-8 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-chlorophenyl)-6-hydroxy-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
i-Pr \\
NH-C-NH \\
i-Pr \\
i-Pr\end{array}$$

RN 168120-33-0 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(4-chloro-3-pyridinyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN <u>168120-34-1</u> HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(4-methyl-2-pyridinyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

IT <u>138046-81-8</u>

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction in prepn. of imidazoles as antiarteriosclerotics)

RN 138046-81-8 HCAPLUS

CN Carbamic acid, (2,4,6-trimethylphenyl)-, phenyl ester (9CI) (CA INDEX NAME)

=> file caold

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
106.97 692.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

CA SUBSCRIBER PRICE -14.55 -16.53

FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004

L8 50 S L7

L9 1575 S L7 FULL

FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004 L10 225 S L9/PREP

```
L11
                 STRUCTURE UPLOADED
L12
             50 S L11
L13
                STRUCTURE UPLOADED
L14
             49 S L13
L15
                 STRUCTURE UPLOADED
L16
              8 S L15
L17
                 STRUCTURE UPLOADED
L18
             50 S L17
                E INDANYL/CN
L19
              1 S E7
                E BENZOFURAN/CN
L20
              1 S E3
                E INDENYL/CN
L21
              1 S E3
L22
                STRUCTURE UPLOADED
L23
             50 S L22
L24
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
           6528 S L24/RCT
L25
L26
             21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                STRUCTURE UPLOADED
L28
             50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
L29
              0 S L26 AND TAN, Z?/AU
L30
              0 S L26 AND SONG, J?/AU
     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
=> s 124 and 19
TOO MANY TERMS FOR FILE CROSSOVER IN L24
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.
=> s 19
L31
            14 L9
```

FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004

=> s 124

TOO MANY TERMS FOR FILE CROSSOVER IN L24

There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> file reg COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.10	694.23
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-16.53

FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

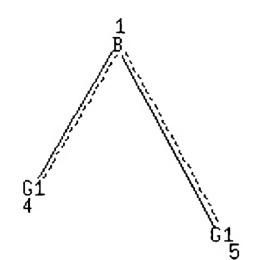
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

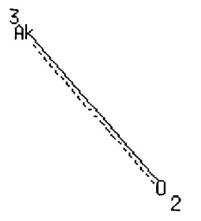
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e 2-amino pyrazole/cn
E1
                    2-AMINO CYCLIC AMP/CN
E2
                    2-AMINO MUSK XYLENE/CN
              0 --> 2-AMINO PYRAZOLE/CN
E3
                    2-AMINO ((METHOXYCARBONYL)THIOUREIDO)BENZENE/CN
\mathbf{E4}
              1
E5
                    2-AMINO(1)BENZOTHIENO(2,3-B)(1)BENZOTHIOPYRAN-11-ONE/CN
E6
                    2-AMINO (HYDRAZONO) METHYL-1, 10-PHENANTHROLINE/CN
              1
E7
                    2-AMINO (PENTAFLUOROETHYL) BENZENE HYDROCHLORIDE/CN
              1
E8
                    2-AMINO-(3-(TERT-BUTYLOXYCARBONYL)PIPERIDIN-1-YL)BENZENE/CN
              1
E9
                    2-AMINO-.ALPHA.,.ALPHA.,5,6-PENTAFLUOROACETOPHENONE/
              1
                    CN
                    2-AMINO-.ALPHA.,.ALPHA.,.ALPHA.-TRIFLUORO-P-TOLUENESULFONAMI
E10
              1
                    DE/CN
E11
                    2-AMINO-.ALPHA.,.ALPHA.,.ALPHA.-TRIFLUORO-P-TOLUENESULFONYL
              1
                    CHLORIDE/CN
E12
                    2-AMINO-.ALPHA.,.ALPHA.,.ALPHA.-TRIFLUOROTOLUENE/CN
              1
=> e amino pyrazole/cn
E1
                    AMINO PEGA RESIN/CN
                    AMINO POLYOL AMINE OXIDASE/CN
E2
E3
                --> AMINO PYRAZOLE/CN
E4
                    AMINO RADICAL/CN
              1
                   AMINO RADICAL (NH2)/CN
E5
              1
                    AMINO SEPHAROSE 6 FAST FLOW/CN
E6
              1
E7
                    AMINO SILOXANES AND SILICONES/CN
              1
                   AMINO TRANSFERASE (STREPTOMYCES COELICOLOR STRAIN A3(2) GENE
E8
             1
                     SCF55.27)/CN
E9
                   AMINO TRANSFERASE (THERMUS THERMOPHILUS STRAIN HB8)/CN
             1
                   AMINO VALERIC ACID/CN
E10
             1
                   AMINO (((2-NITROPHENYL)METHYL)AMINO)METHANE-1-THIONE/CN
E11
             1
                   AMINO ((3,4-DICHLOROPHENYL) AMINO) METHANE-1-THIONE/CN
E12
             1
=>
L32
        STRUCTURE UPLOADED
=> d 132
L32 HAS NO ANSWERS
L32
                STR
Ak & 0 M1 X 8
```

Page 1-A



Page 1-B



Page 2-B

VAR G1=6/7/8/2 NODE ATTRIBUTES:

HCOUNT IS M1 AT**NSPEC** IS C AT1 NSPEC IS C AT**NSPEC** IS C TA3 **NSPEC** IS C AT 4 **NSPEC** IS C 5 ATDEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 1 2 3 6 7 8

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

=> s 132

SAMPLE SEARCH INITIATED 10:23:58 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 16360 TO ITERATE

6.1% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

PROJECTED ITERATIONS: BATCH **COMPLETE**

319545 TO 334855

PROJECTED ANSWERS:

50 SEA SSS SAM L32

=> s 132 full

L33

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 10:24:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 327382 TO ITERATE

79883 TO 87643

100.0% PROCESSED 327382 ITERATIONS SEARCH TIME: 00.00.04

89725 ANSWERS

SESSION

-16.53

ENTRY

0.00

L34 89725 SEA SSS FUL L32

CA SUBSCRIBER PRICE

=> file hcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
159.20 853.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 134/rct 117519 L34

2633407 RCT/RL

L35 36779 L34/RCT

(L34 (L) RCT/RL)

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004 L7 STRUCTURE UPLOADED

```
FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
 L8
              50 S L7
 L9
            1575 S L7 FULL
      FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
             225 S L9/PREP
 L10
      FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
 L11
                 STRUCTURE UPLOADED
 L12
              50 S L11
L13
                 STRUCTURE UPLOADED
L14
              49 S L13
L15
                 STRUCTURE UPLOADED
L16
               8 S L15
                 STRUCTURE UPLOADED
L17
L18
              50 S L17
                 E INDANYL/CN
L19
               1 S E7
                 E BENZOFURAN/CN
L20
               1 S E3
                 E INDENYL/CN
L21
               1 S E3
L22
                 STRUCTURE UPLOADED
L23
              50 S L22
L24
           65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
L25
            6528 S L24/RCT
L26
              21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                 STRUCTURE UPLOADED
L28
             50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
              0 S L26 AND TAN, Z?/AU
L29
              0 S L26 AND SONG, J?/AU
L30
     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
L31
             14 S L9
     FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004
                E 2-AMINO PYRAZOLE/CN
                E AMINO PYRAZOLE/CN
                STRUCTURE UPLOADED
L32
L33
             50 S L32
L34
          89725 S L32 FULL
     FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
          36779 S L34/RCT
L35
=> d his
     (FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)
     FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004
     FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004
L1
                STRUCTURE UPLOADED
```

```
L2
               0 S L1
 L3
               0 S L1 FULL
L4
                 STRUCTURE UPLOADED
L5
               0 S L4
L_6
               3 S L4 FULL
      FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
                 STRUCTURE UPLOADED
L7
      FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
\Gamma8
              50 S L7
L9
            1575 S L7 FULL
      FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
L10
             225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                 STRUCTURE UPLOADED
L12
              50 S L11
                 STRUCTURE UPLOADED
L13
L14
              49 S L13
L15
                 STRUCTURE UPLOADED
L16
               8 S L15
L17
                 STRUCTURE UPLOADED
L18
              50 S L17
                 E INDANYL/CN
L19
               1 S E7
                 E BENZOFURAN/CN
L20
               1 S E3
                 E INDENYL/CN
L21
               1 S E3
                 STRUCTURE UPLOADED
L22
L23
              50 S L22
L24
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
           6528 S L24/RCT
L25
             21 S L25 AND L10
L26
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                 STRUCTURE UPLOADED
L28
              50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
L29
              0 S L26 AND TAN, Z?/AU
L30
              0 S L26 AND SONG, J?/AU
     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
L31
             14 S L9
     FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004
                E 2-AMINO PYRAZOLE/CN
                E AMINO PYRAZOLE/CN
L32
                STRUCTURE UPLOADED
L33
             50 S L32
L34
          89725 S L32 FULL
     FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
          36779 S L34/RCT
L35
```

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004

L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004

L8 50 S L7

L9 1575 S L7 FULL

FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004

L10 225 S L9/PREP

FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004

L11 STRUCTURE UPLOADED

L12 50 S L11

L13 STRUCTURE UPLOADED

L14 49 S L13

L15 STRUCTURE UPLOADED

L16 8 S L15

L17 STRUCTURE UPLOADED

L18 50 S L17

E INDANYL/CN

L19 1 S E7

E BENZOFURAN/CN

L20 1 S E3

E INDENYL/CN

L21 1 S E3

L22 STRUCTURE UPLOADED

L23 50 S L22

L24 65845 S L22 FULL

FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004

L25 6528 S L24/RCT

L26 21 S L25 AND L10

FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004

L27 STRUCTURE UPLOADED

L28 50 S L27

FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004

L29 0 S L26 AND TAN, Z?/AU

L30 0 S L26 AND SONG, J?/AU

FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004

L31 14 S L9

FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004 E 2-AMINO PYRAZOLE/CN

```
E AMINO PYRAZOLE/CN
L32
                 STRUCTURE UPLOADED
L33
             50 S L32
L34
          89725 S L32 FULL
     FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
L35
          36779 S L34/RCT
=> s 135 and 126
L36
             1 L35 AND L26
=> d 136, ibib abs, 1
     ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
L36
   Full
            Citing
   Text
          References
ACCESSION NUMBER:
                          2000:666713 HCAPLUS
DOCUMENT NUMBER:
                          133:252426
                          Preparation of aromatic heterocyclic ureas as
TITLE:
                          antiinflammatory agents
INVENTOR(S):
                          Betageri, Rajashehar; Breitfelder, Steffen; Cirillo,
                          Pier F.; Gilmore, Thomas A.; Hickey, Eugene R.;
                          Kirrane, Thomas M.; Moriak, Monica H.; Moss, Neil;
                          Patel, Usha R.; Proudfoot, John R.; Regan, John R.;
                          Sharma, Rajiv; Sun, Sanxing; Swinamer, Alan D.;
                          Takahashi, Hidenori
                          Boehringer Ingelheim Pharmaceuticals, Inc., USA
PATENT ASSIGNEE(S):
SOURCE:
                          PCT Int. Appl., 282 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:
                          Patent
LANGUAGE:
                          English
FAMILY ACC. NUM. COUNT:
                          3
PATENT INFORMATION:
     PATENT NO.
                      KIND
                            DATE
                                            APPLICATION NO.
                                                              DATE
     WO 2000055139
                       A2
                             20000921
                                            WO 2000-US3865
                                                              20000216
     WO 2000055139
                       Α3
                             20010426
             AE, AU, BG, BR, BY, CA, CN, CZ, EE, HR, HU, ID, IL, IN, JP, KR,
             KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, VN,
             YU, ZA
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     EP 1165516
                       A2
                             20020102
                                            EP 2000-907295
                                                              20000216
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
    BR 2000008922
                       Α
                            20020115
                                            BR 2000-8922
                                                              20000216
    TR 200102817
                       T2
                            20020521
                                            TR 2001-20010281720000216
    JP 2002539198
                       T2
                            20021119
                                            JP 2000-605569
                                                              20000216
    EE 200100483
                       A
                            20021216
                                            EE 2001-483
                                                              20000216
    NZ 514711
                       Α
                            20040227
                                            NZ 2000-514711
                                                              20000216
    AU 771273
                       B2
                            20040318
                                            AU 2000-28817
                                                              20000216
    BG 105880
                       Α
                                            BG 2001-105880
                            20020531
                                                              20010905
```

20020910

20030630

20010911

20020509

20031209

20020627

20031202

ZA 2001-7446

HR 2001-665

NO 2001-4412

<u>US</u> 2001-962709

US 2001-962057

20010910

20010910

20010911

20010925

20010925

ZA 2001007446

HR 2001000665

NO 2001004412

US 2002055507

US 2002082256

US 6660732

US 6656933

Α

A1

Α

A1

B2

Α1

B2

US 2003225077 US 2003-424613 20031204 A120030428 US 2004019038 A1 20040129 US 2003-624289 20030721 PRIORITY APPLN. INFO.: US 1999-124148P 19990312 US 1999-165867P 19991116 US 2000-505582 A3 20000216 WO 2000-US3865 20000216 US 2001-962057 A1 20010925 US 2001-962709 A3 20010925

MARPAT 133:252426

ΙΙ

OTHER SOURCE(S):

GI

The title compds. (I) [wherein Ar1 = (un) substituted pyrrole, pyrrolidine, ABpyrazole, imidazole, oxazole, thiazole, furan, or thiophene; Ar2 = (un) substituted Ph, (tetrahydro) naphthyl, (tetrahydro) quinoline, (tetrahydro)isoquinoline, benzimidazole, benzofuran, indanyl, indenyl, or indole; W = O or S; X = (un) substituted cycloalkyl, cycloalkenyl, Ph, furan, thiophene, pyrrole, imidazolyl, pyridine, pyrimidine, (dihydro)pyridinone, (dihydro)maleimide, piperidine, piperazine, or pyrazine; Y = a bond or (un) substituted satd. or unsatd. alkyl optionally interrupted by O, NH, S(O), SO2, or S; Z = (un) substituted Ph, pyridine, pyrimidine, pyridazine, imidazole, (tetrahydro) furan, thiophene, (tetrahydro)pyran, 1,3-dioxolanone, 1,3-dioxanone, 1,4-dioxane, (thio) morpholine (sulfoxide), piperidine, cyclohexanone, pentamethylene sulfoxide, etc.] were prepd. for the treatment of diseases or pathol. conditions involving inflammation, such as chronic inflammatory diseases. Thus, coupling 2-cyclohexenone with 4-bromo-1-naphthylamine in the presence of Pd(PPh3)2Cl2, DPPP, and NaHCO3 in DMF, followed by conversion of the amine to an isocyanate using ClCOCl and immediate addn. of 1-(4-methylphenyl)-3-tert-butyl-1H-pyrazol-5-amine, gave the urea II. a cytokine prodn. inhibition assay, preferred compds. of the invention showed IC50 < 10 μM against TNF- α in lipopolysaccharide stimulated THF cells.

=> file caold COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 16.70 870.13 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE

TOTAL SESSION

CA SUBSCRIBER PRICE

ENTRY -0.69

-17.22

FILE 'CAOLD' ENTERED AT 10:28:13 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

STRUCTURE UPLOADED L1

L20 S L1

L30 S L1 FULL

L4STRUCTURE UPLOADED

L5 0 S L4

3 S L4 FULL L6

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004

L850 S L7

L9 1575 S L7 FULL

FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004 225 S L9/PREP L10

FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004

L11STRUCTURE UPLOADED

L12 50 S L11

L13 STRUCTURE UPLOADED

L1449 S L13

L15 STRUCTURE UPLOADED

L16 8 S L15

L17 STRUCTURE UPLOADED

L18 50 S L17

E INDANYL/CN

L19 1 S E7

E BENZOFURAN/CN

L20 1 S E3

L21 1 S E3 L22STRUCTURE UPLOADED L2350 S L22 L2465845 S L22 FULL FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004 6528 S L24/RCT L25L26 21 S L25 AND L10 FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004 L27 STRUCTURE UPLOADED L28 50 S L27 FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004 L29 0 S L26 AND TAN, Z?/AU L30 0 S L26 AND SONG, J?/AU FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004 L31 14 S L9 FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004 E 2-AMINO PYRAZOLE/CN E AMINO PYRAZOLE/CN L32 STRUCTURE UPLOADED L33 50 S L32 L3489725 S L32 FULL FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004 36779 S L34/RCT L35 L36 1 S L35 AND L26 FILE 'CAOLD' ENTERED AT 10:28:13 ON 24 JUN 2004 => s 134 and 19 TOO MANY TERMS FOR FILE CROSSOVER IN L34 There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information. => s 19 and 134 TOO MANY TERMS FOR FILE CROSSOVER IN L34 There are limits on the size of an answer set being crossed over from one file to another. Enter HELP_CROSSOVER at an arrow prompt (=>) for specific information. => s 131 and base 9375 BASE 6467 BASES 15700 BASE (BASE OR BASES) L37 0 L31 AND BASE => file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 5.51 875.64 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

E INDENYL/CN

CA SUBSCRIBER PRICE

0.00 -17.22

FILE 'REGISTRY' ENTERED AT 10:33:49 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

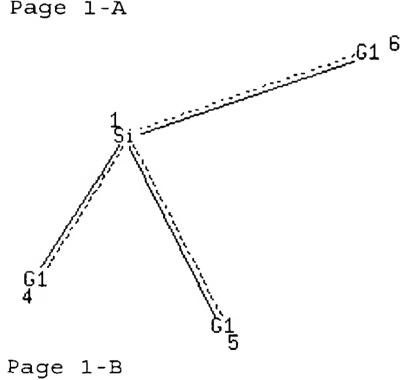
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

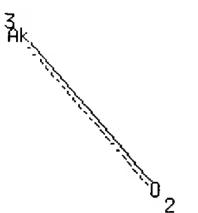
=>

L38 STRUCTURE UPLOADED

=> d 138 L38 HAS NO ANSWERS L38 STR

Ak 8 0 M1 X 9 Page 1-A





Page 2-B VAR G1=7/8/9/2 NODE ATTRIBUTES: HCOUNT IS M1

AT 8

```
NSPEC
       IS C
                  {
m AT}
                        1
NSPEC
        IS C
                  AT
                        2
NSPEC
        IS C
                  \mathsf{AT}
NSPEC
       IS C
                  \mathtt{AT}
NSPEC
       IS C
                   \mathsf{AT}
                        5
NSPEC
        IS C
                   \mathtt{AT}
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
                        1 2 3 7 8 9
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
=> s 138
SAMPLE SEARCH INITIATED 10:35:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 55513 TO ITERATE
  1.8% PROCESSED
                     1000 ITERATIONS
                                                                50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
                         BATCH
                                 **INCOMPLETE**
PROJECTED ITERATIONS:
                           EXCEEDS 1000000
                          EXCEEDS 584795
PROJECTED ANSWERS:
L39
             50 SEA SSS SAM L38
=> e silicon/cn
E1
                    SILICOMOLYBDOVANADIC ACID (H6M010SIV2040)/CN
E2
                   SILICOMONAZITE/CN
            1 --> SILICON/CN
E3
                   SILICON (DIPHOSPHATE)/CN
E4
             1
                   SILICON (SI(3+))/CN
E5
             1
                   SILICON (SI10+) CLUSTER ION/CN
E6
             1
                   SILICON (SI11+) CLUSTER ION/CN
Ε7
                   SILICON (SI12+) CLUSTER ION/CN
E8
             1
                   SILICON (SI13+) CLUSTER ION/CN
E9
E10
                   SILICON (SI14+) CLUSTER ION/CN
             1
                   SILICON (SI15+) CLUSTER ION/CN
E11
             1
                   SILICON (SI16+) CLUSTER ION/CN
E12
=> s e3
             1 SILICON/CN
L40
=> d 13
L3 HAS NO ANSWERS
L1
                STR
L3
              O SEA FILE=CASREACT SSS FUL L1 (
                                                    0 REACTIONS)
=> d his
     (FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)
```

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

```
FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004
 L1
                 STRUCTURE UPLOADED
 L2
               0 S L1
 L3
               0 S L1 FULL
                 STRUCTURE UPLOADED
 L4
 L5
               0 S L4
 L6
               3 S L4 FULL
      FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
                 STRUCTURE UPLOADED
L7
      FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
L8
              50 S L7
L9
            1575 S L7 FULL
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
             225 S L9/PREP
L10
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                 STRUCTURE UPLOADED
L12
              50 S L11
L13
                 STRUCTURE UPLOADED
L14
              49 S L13
                 STRUCTURE UPLOADED
L15
L16
               8 S L15
                 STRUCTURE UPLOADED
L17
L18
              50 S L17
                 E INDANYL/CN
L19
               1 S E7
                 E BENZOFURAN/CN
L20
               1 S E3
                 E INDENYL/CN
L21
               1 S E3
L22
                 STRUCTURE UPLOADED
L23
              50 S L22
L24
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
L25
           6528 S L24/RCT
             21 S L25 AND L10
L26
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                 STRUCTURE UPLOADED
L28
             50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
L29
              0 S L26 AND TAN, Z?/AU
L30
              0 S L26 AND SONG, J?/AU
     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
L31
             14 S L9
     FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004
                E 2-AMINO PYRAZOLE/CN
                E AMINO PYRAZOLE/CN
L32
                STRUCTURE UPLOADED
L33
             50 S L32
          89725 S L32 FULL
L34
```

FILE	'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
	36779 S L34/RCT
	1 S L35 AND L26
FILE	'CAOLD' ENTERED AT 10:28:13 ON 24 JUN 2004
	0 S L31 AND BASE
FILE	'REGISTRY' ENTERED AT 10:33:49 ON 24 JUN 2004
	STRUCTURE UPLOADED
	50 S L38
	E SILICON/CN
	1 S E3
	FILE

=>

Patent Assignment Abstract of Title

Total Assignments: 1

Application #: 10074895 **Filing Dt:** 02/12/2002 Patent #: NONE Issue Dt:

PCT #: NONE Publication #: <u>US20020123631</u> Pub Dt: 09/05/

Inventors: Zhulin Tan, Jinhua J. Song

Process for synthesis of heteroaryl-substituted urea compounds useful as antiinflammatory agents

Assignment: 1

Reel/Frame: 012594/0147 Received: 02/26/2002 Recorded: 02/12/2002 Mailed: 04/17/2002 Pag

Conveyance: ASSIGNMENT OF ASSIGNORS INTEREST (SEE DOCUMENT FOR DETAILS).

Assignors: TAN, ZHULIN **Exec Dt:** 01/17/2002

> SONG, JINHUA J. Exec Dt: 01/17/2002

Assignee: BOEHRINGER INGELHEIM PHARMACEUTICALS, INC.

P.O. BOX 368

900 RIDGEBURY ROAD

RIDGEFIELD, CONNECTICUT 06877

Correspondent: BOEHRINGER INGELHEIM CORPORATION

ROBERT P. RAYMOND 900 RIDGEBURY ROAD

P.O. BOX 368

RIDGEFIELD, CT 06877-0368

Search Results as of: 6/20/2004 10:47:05 P.M.